

## **SUPPLEMENTARY INFORMATION. 2**

### **The most reactive amide as a transition state mimic for *cis-trans* interconversion.**

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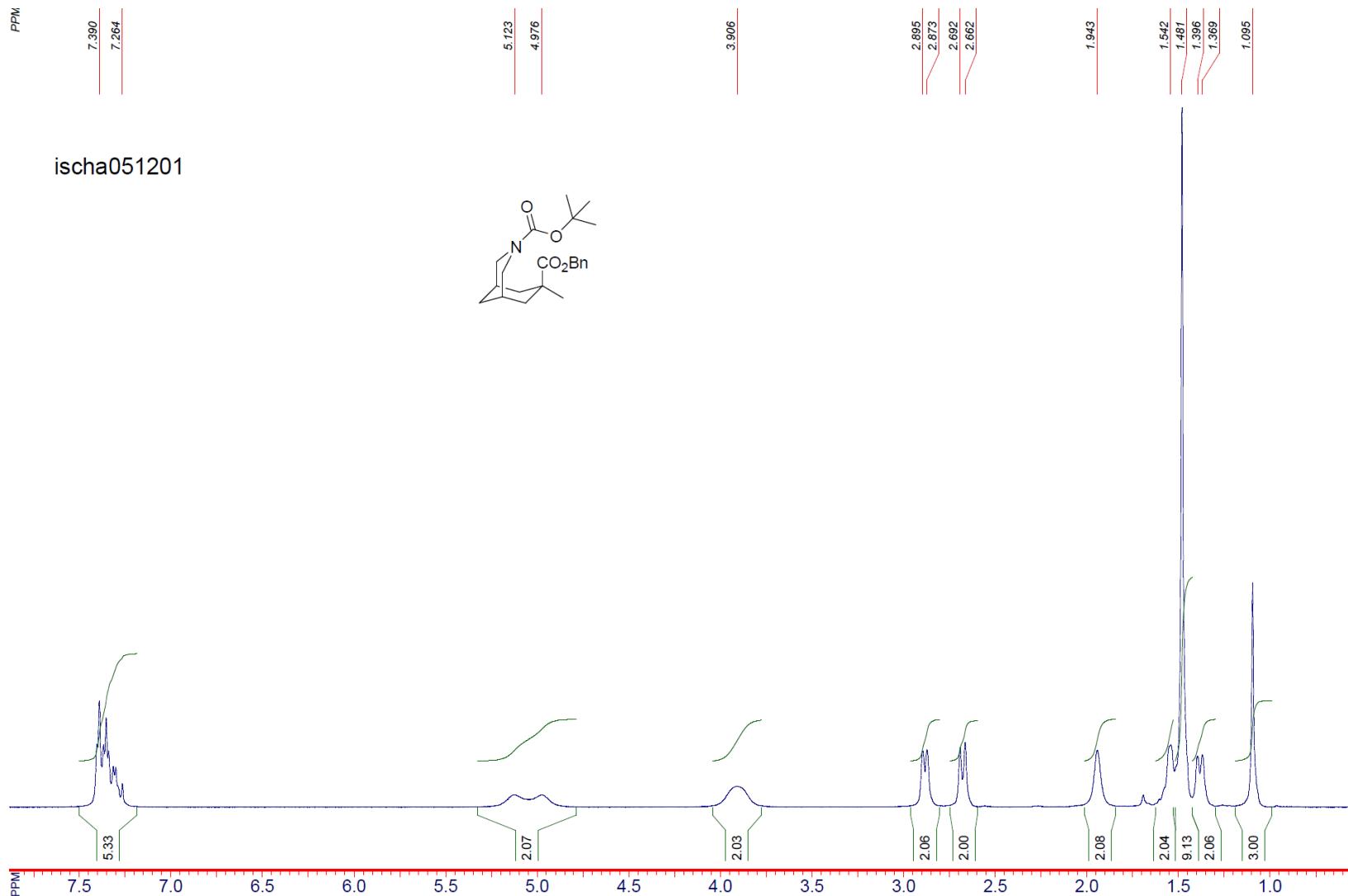
\* Corresponding authors. E-mail: ajk1@cam.ac.uk (AJK); ik214@yahoo.com (IVK).

**S.5 Spectroscopic Data.**

**NMR and Mass spectra**

**S.45 – S.72**

PPM



$^1\text{H}$ -NMR spectrum of **19** ( $\text{CDCl}_3$ , 500 MHz).

PPM

175.92

156.22

136.45

128.00  
127.97  
127.44

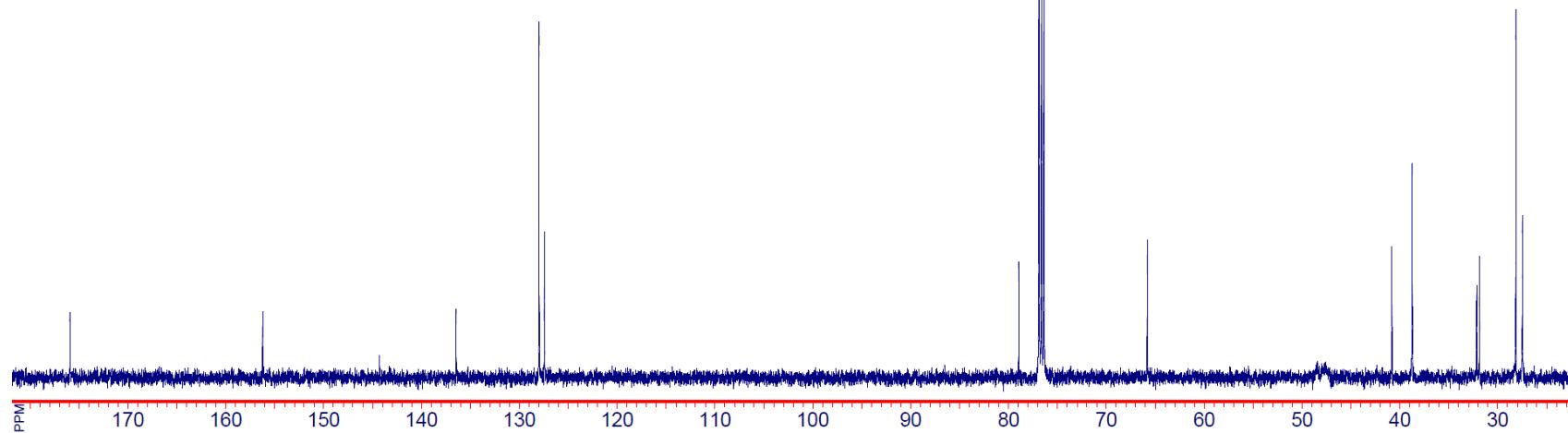
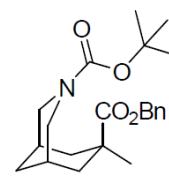
78.97

65.83

40.84  
38.77

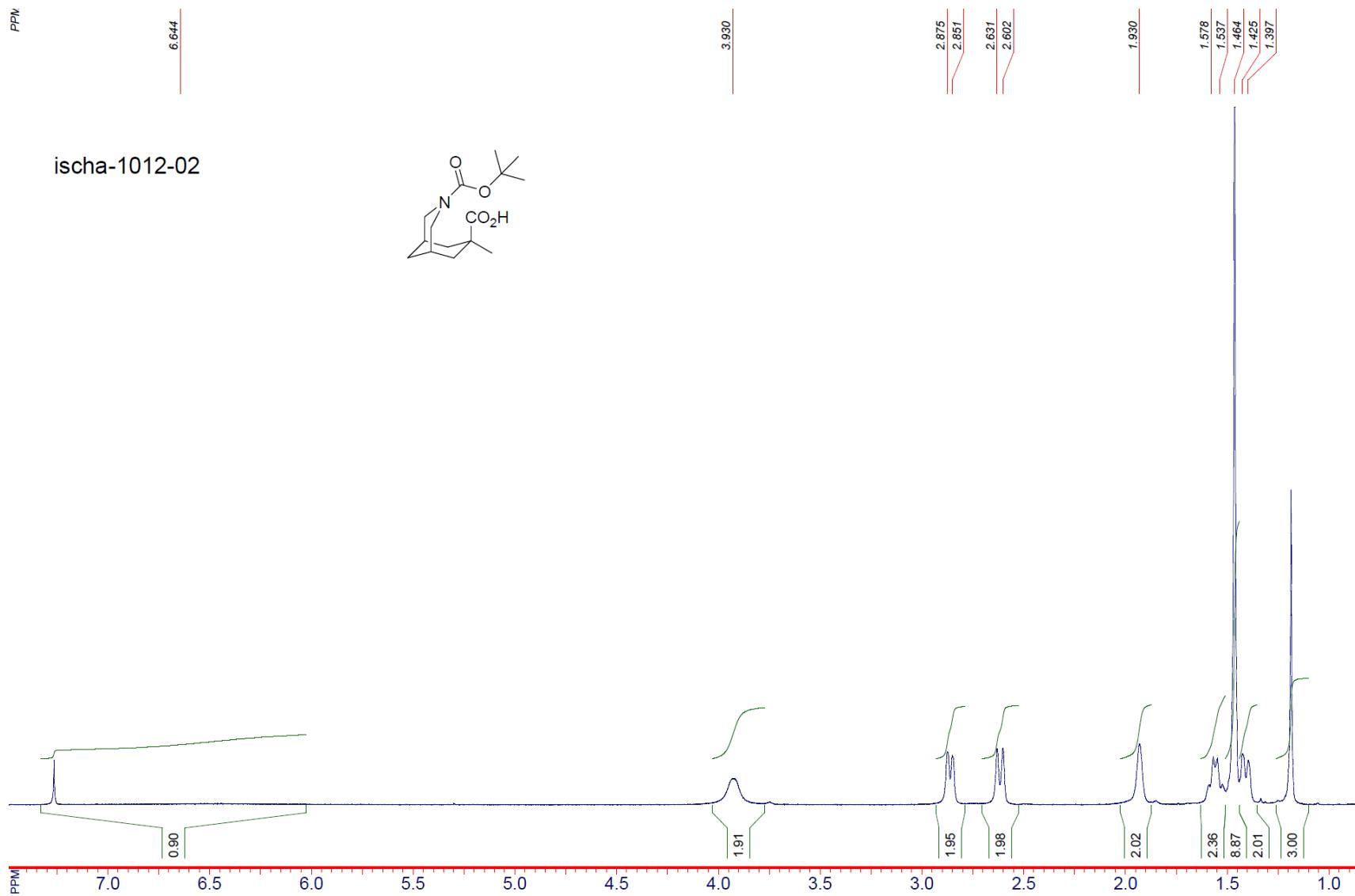
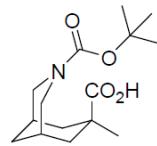
32.16  
31.88  
28.16  
27.50

ischa051201\_C13



$^{13}\text{C}$ -NMR spectrum of **19** ( $\text{CDCl}_3$ , 124.9 MHz).

ischa-1012-02



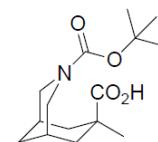
$^1\text{H}$ -NMR spectrum of **20** ( $\text{CDCl}_3$ , 500 MHz).

PPM

176.61

155.61

ischa-1012-02\_C13



PPM

47.78

40.14

38.76

32.20  
32.08

28.13

27.47

79.11

47.78

40.14

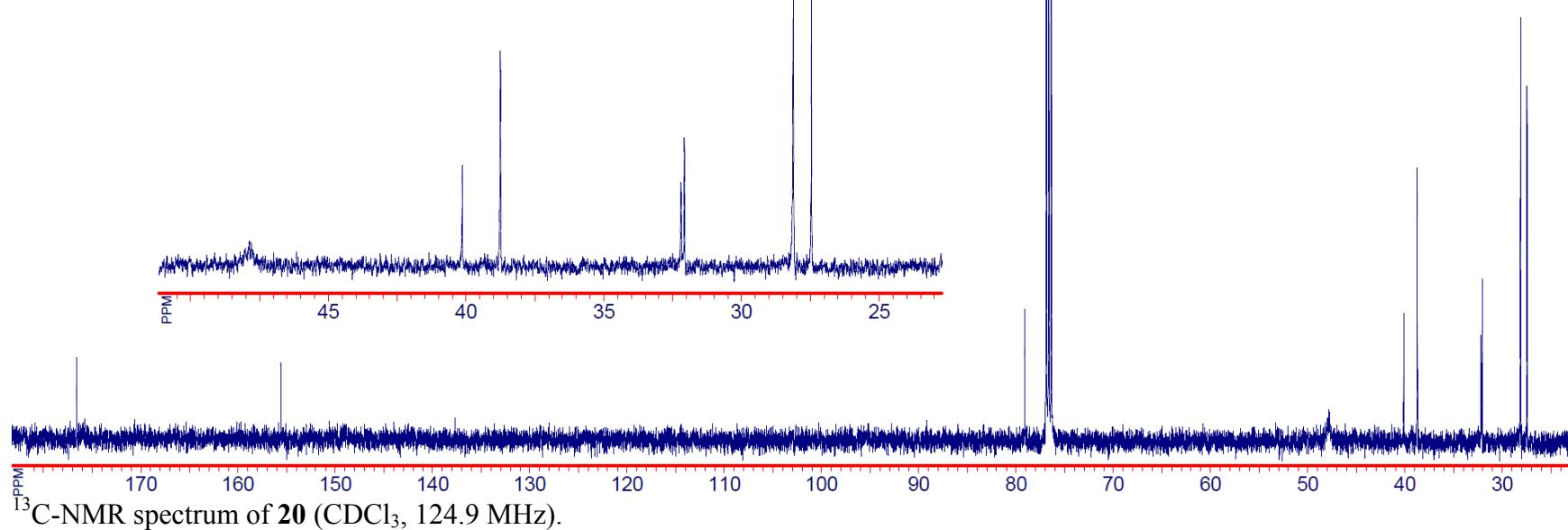
38.76

32.20

32.08

28.13

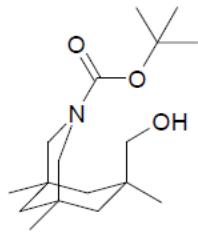
27.47



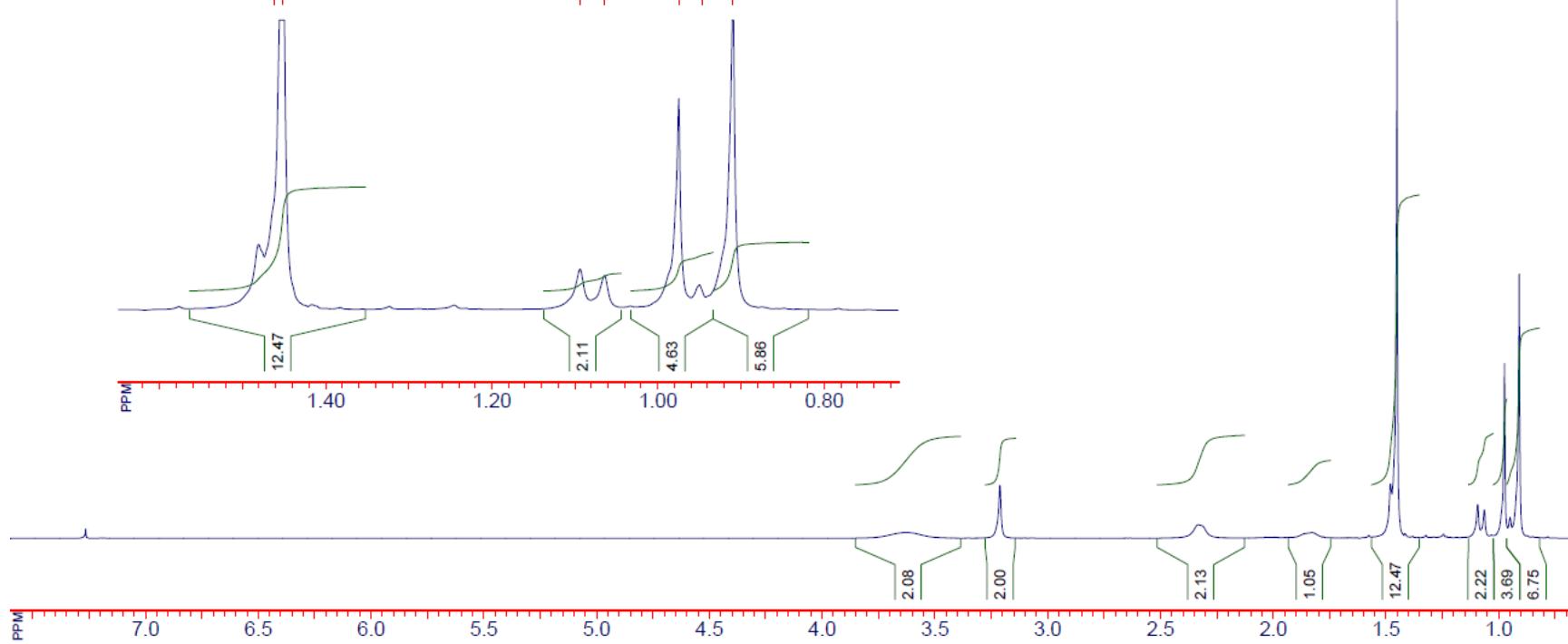
<sup>13</sup>C-NMR spectrum of **20** ( $\text{CDCl}_3$ , 124.9 MHz).

PPM

komta-5-2



PPM

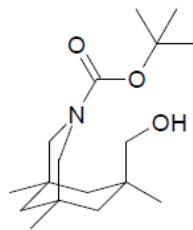


<sup>1</sup>H-NMR spectrum of **21** (CDCl<sub>3</sub>, 500 MHz).

PPM

155.68

komta-5-2\_C13



79.23

72.23

55.43

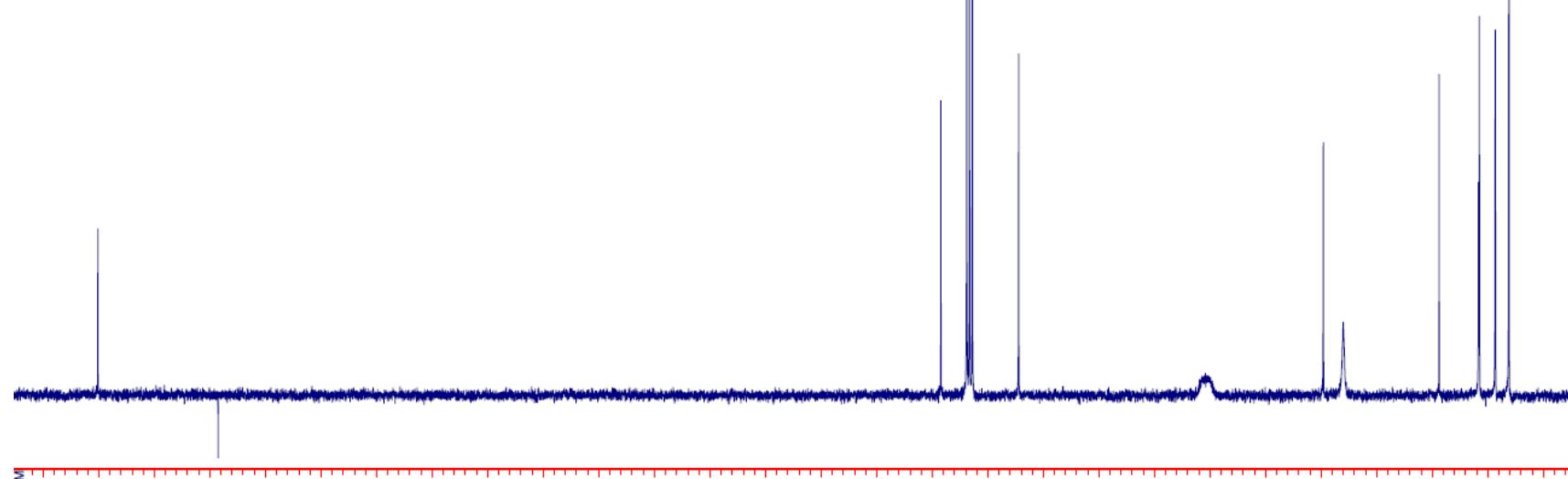
44.82

34.40

30.78

29.35

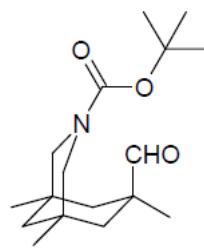
28.12



<sup>13</sup>C-NMR spectrum of **21** (CDCl<sub>3</sub>, 124.9 MHz).

PPM

9.172



komta-6-2

PPM

2.354

2.329

2.150

2.125

1.461

1.104

1.072

0.901

0.830

3.566

2.354

2.329

2.150

2.125

1.461

1.104

1.072

0.901

0.830

PPM

2.15

2.10

10.48

4.49

6.55

3.41

2.07

2.15

2.10

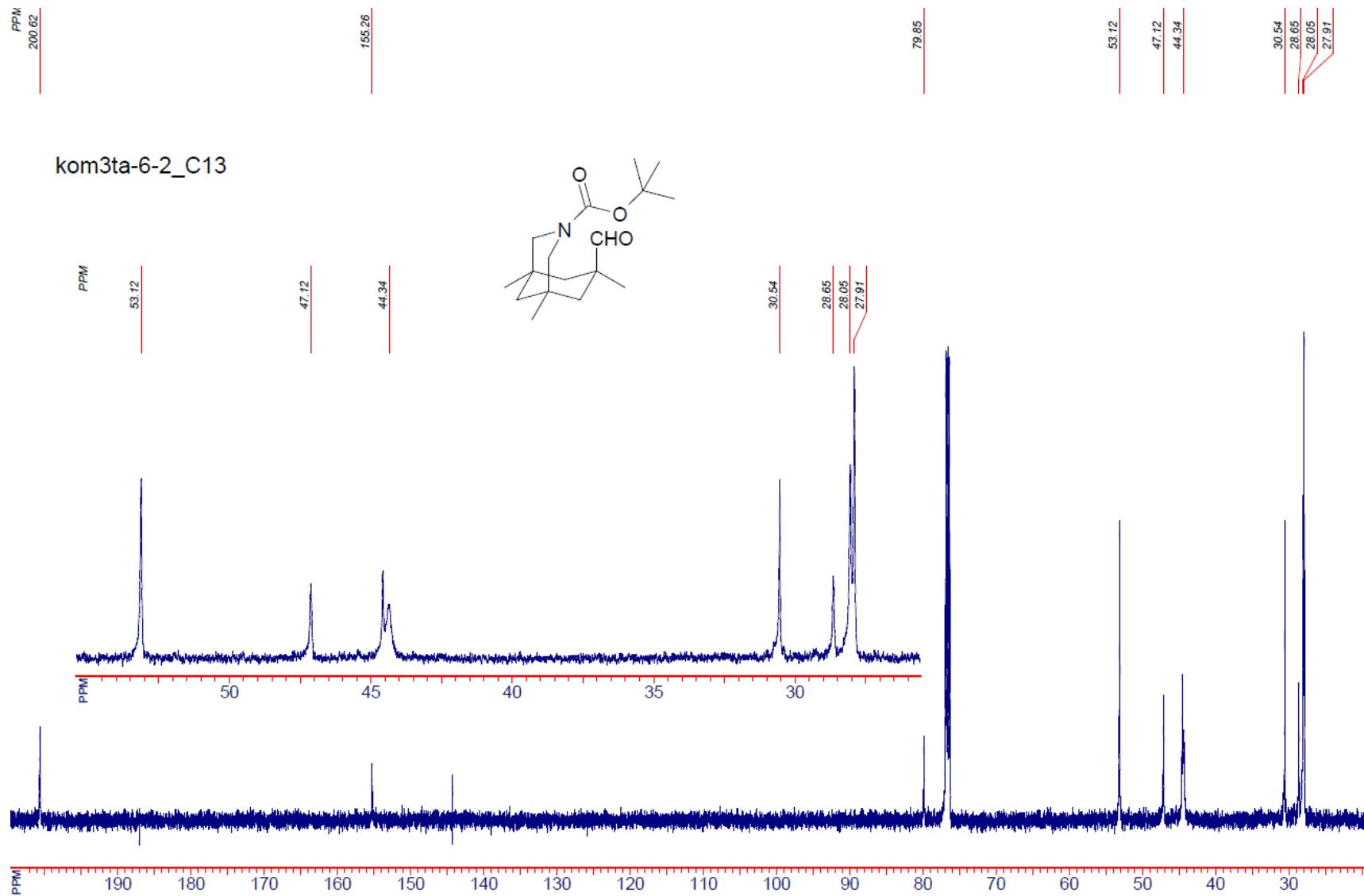
10.48

4.49

6.55

3.41

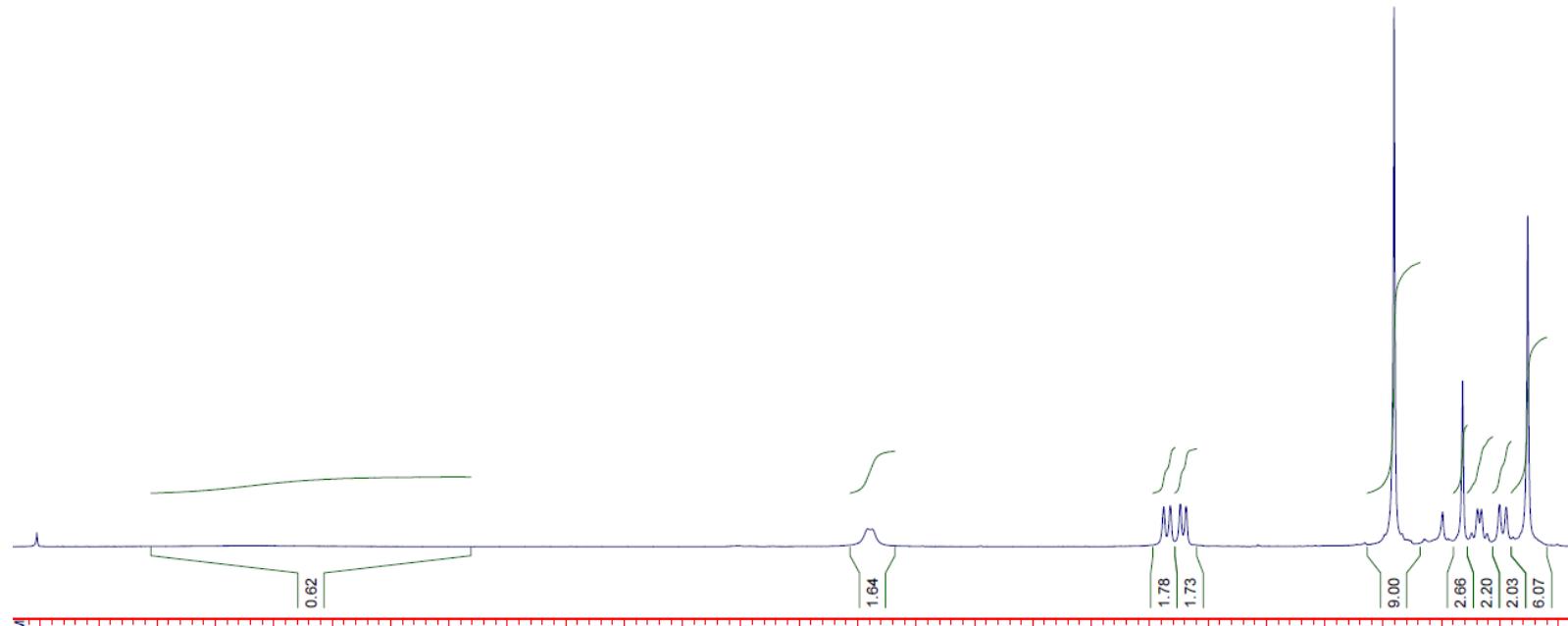
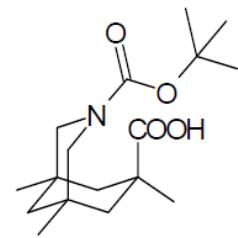
<sup>1</sup>H-NMR spectrum of 23 (CDCl<sub>3</sub>, 500 MHz).



<sup>13</sup>C-NMR spectrum of **23** ( $\text{CDCl}_3$ , 124.9 MHz).

PPM

komta-7-2



$^1\text{H}$ -NMR spectrum of **24** ( $\text{CDCl}_3$ , 500 MHz).

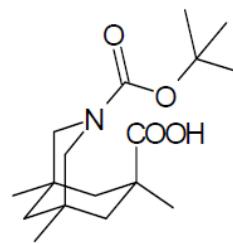
PPM

PPM

176.39

155.36

komta-7-2 C13



79.28

52.91

47.24

45.33

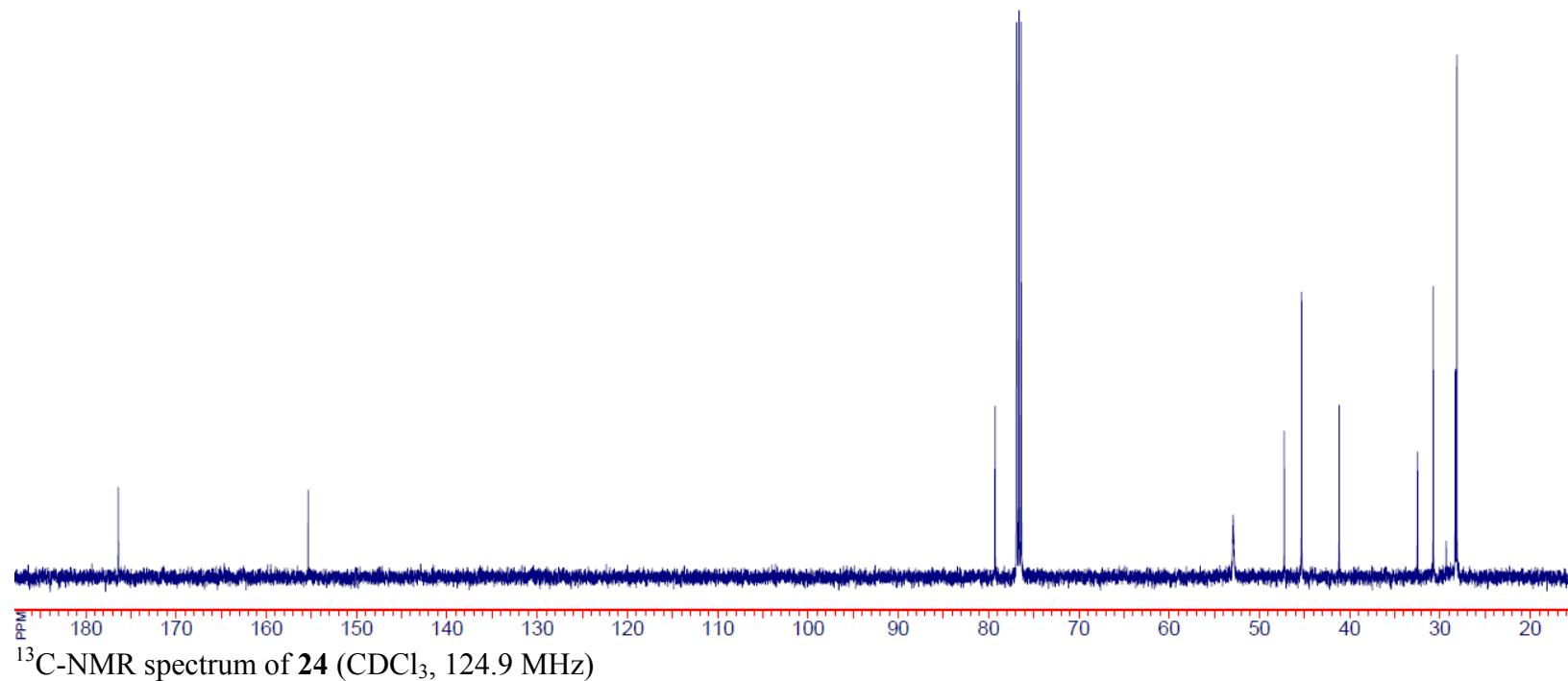
41.16

32.49

30.75

29.31

28.14

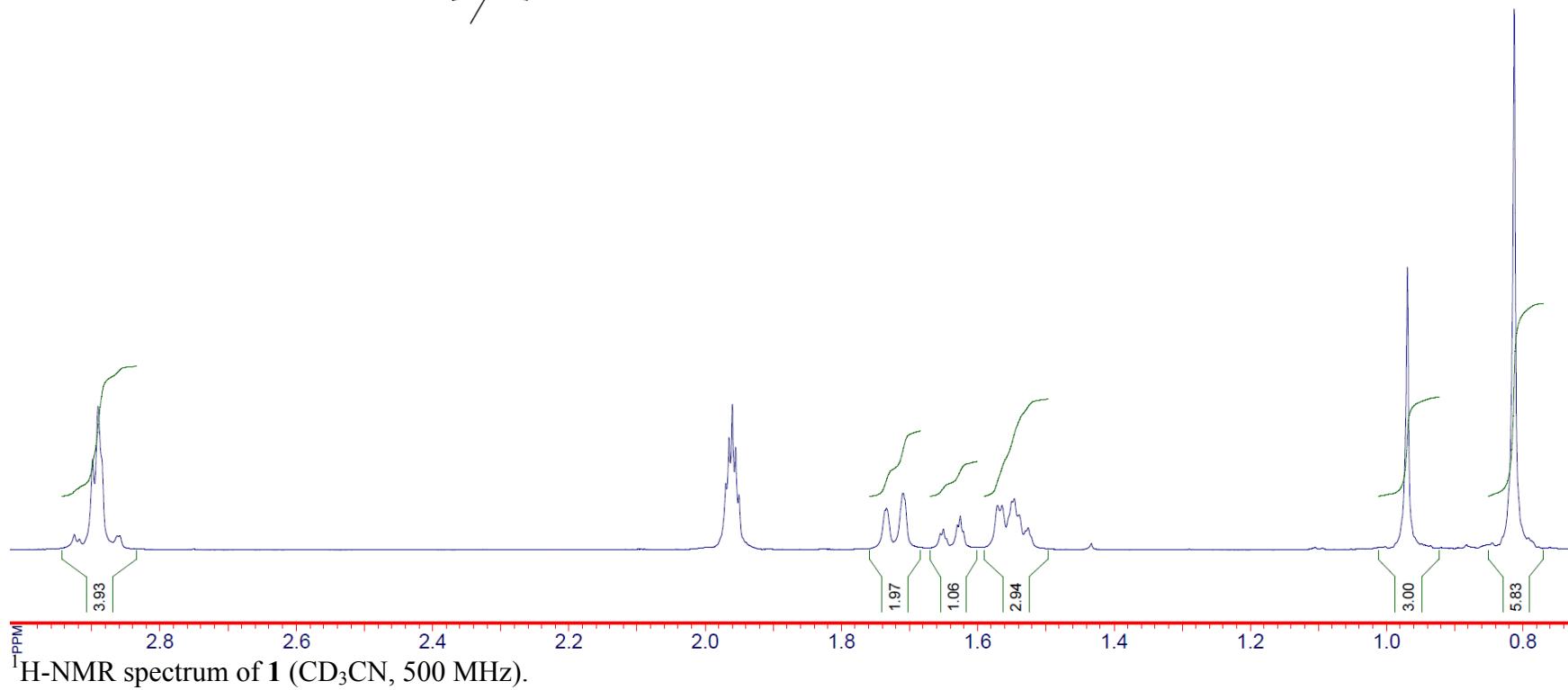
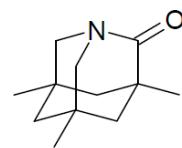


<sup>13</sup>C-NMR spectrum of **24** ( $\text{CDCl}_3$ , 124.9 MHz)

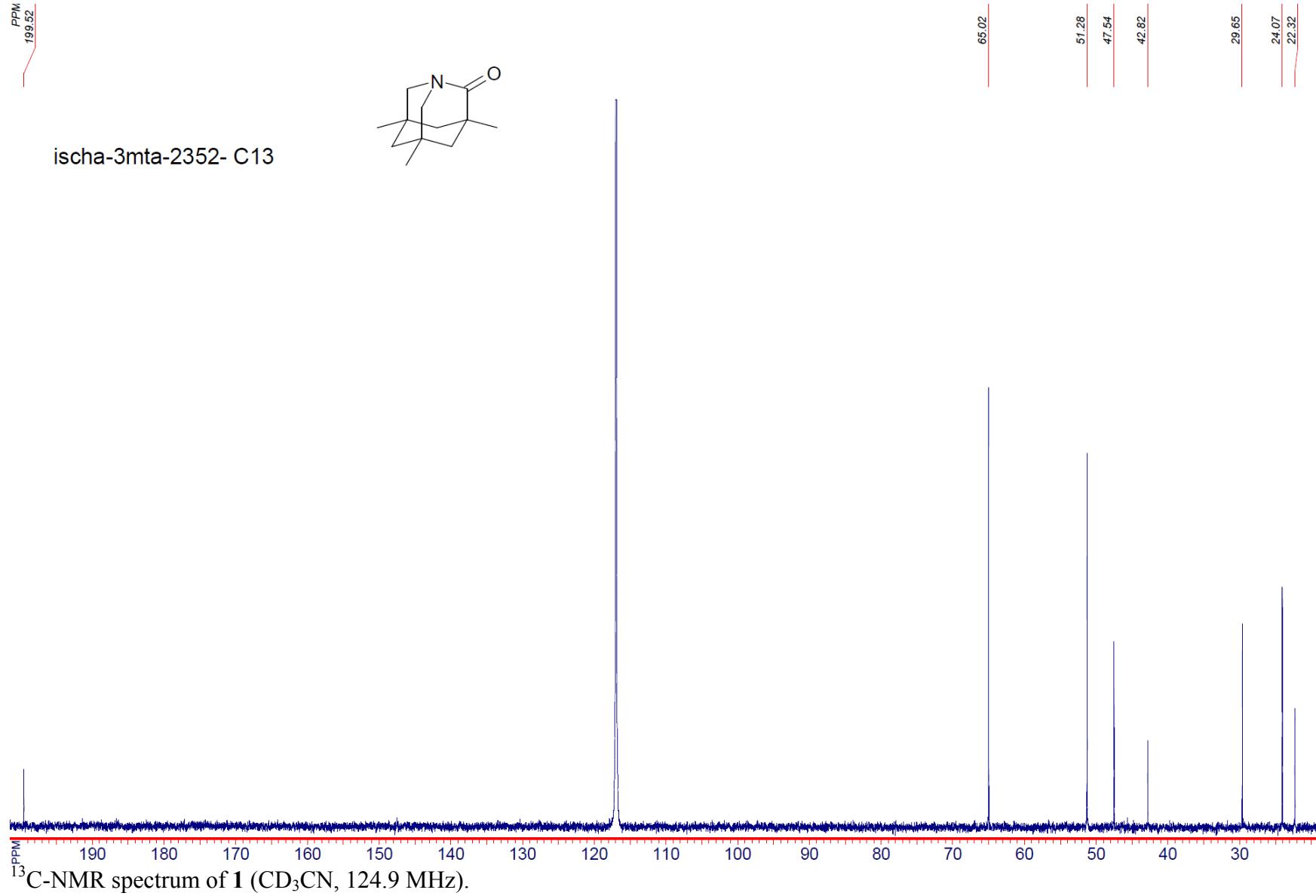
PPM

2.926  
2.918  
2.899  
2.890  
2.887  
2.862  
2.859

ischa-3mta

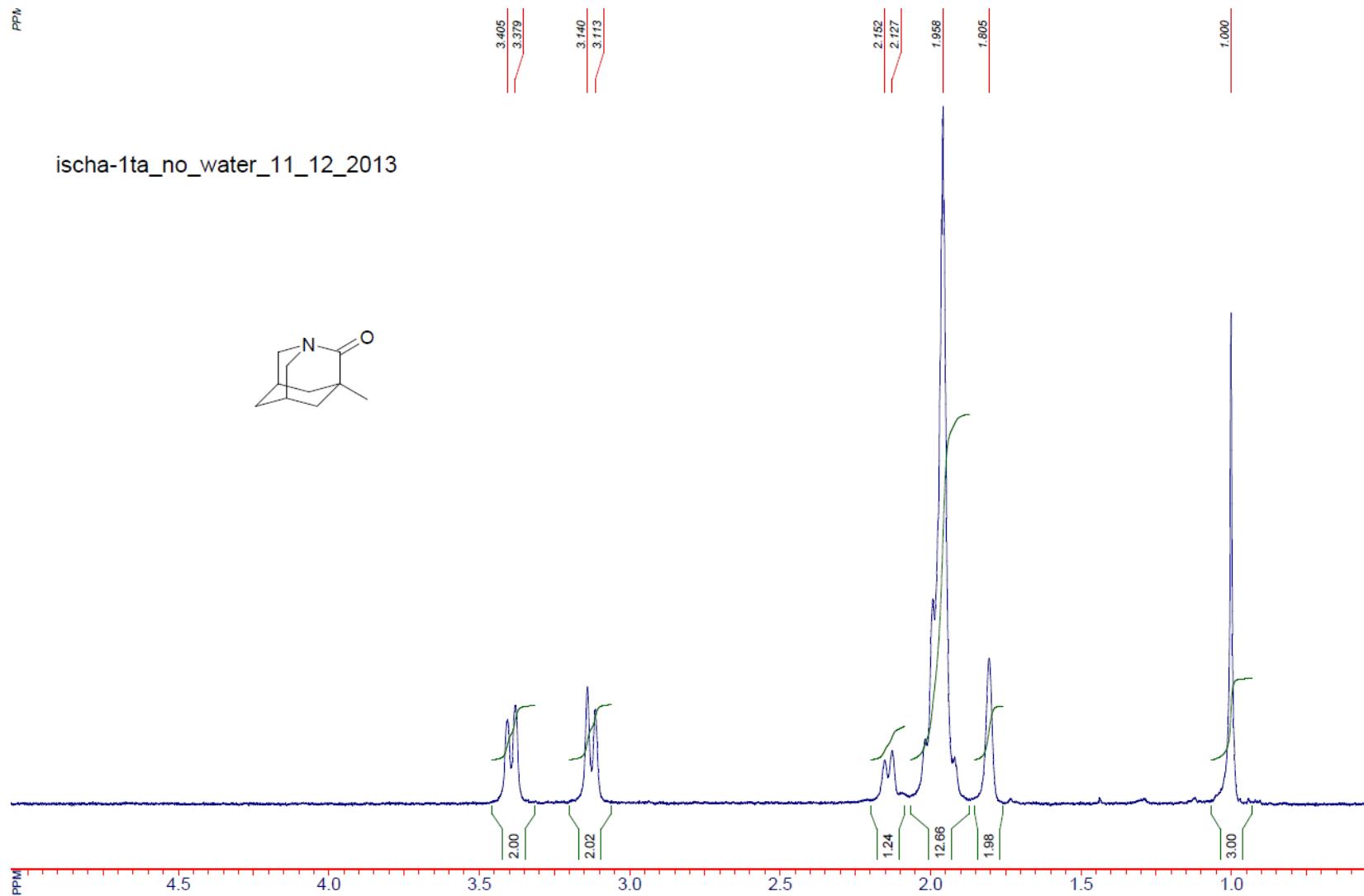
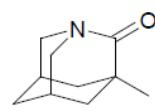


<sup>1</sup>H-NMR spectrum of **1** (CD<sub>3</sub>CN, 500 MHz).

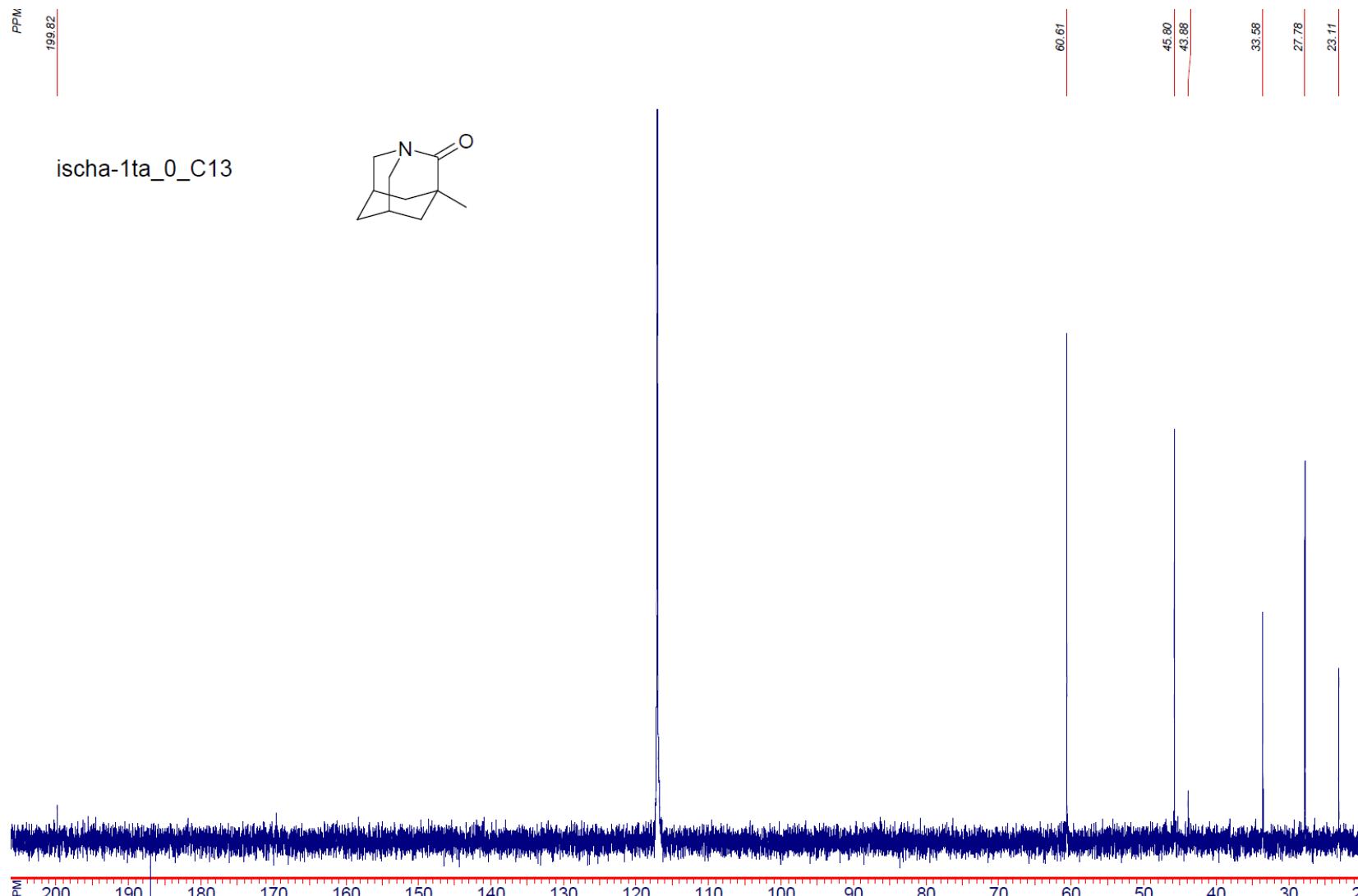


PPM

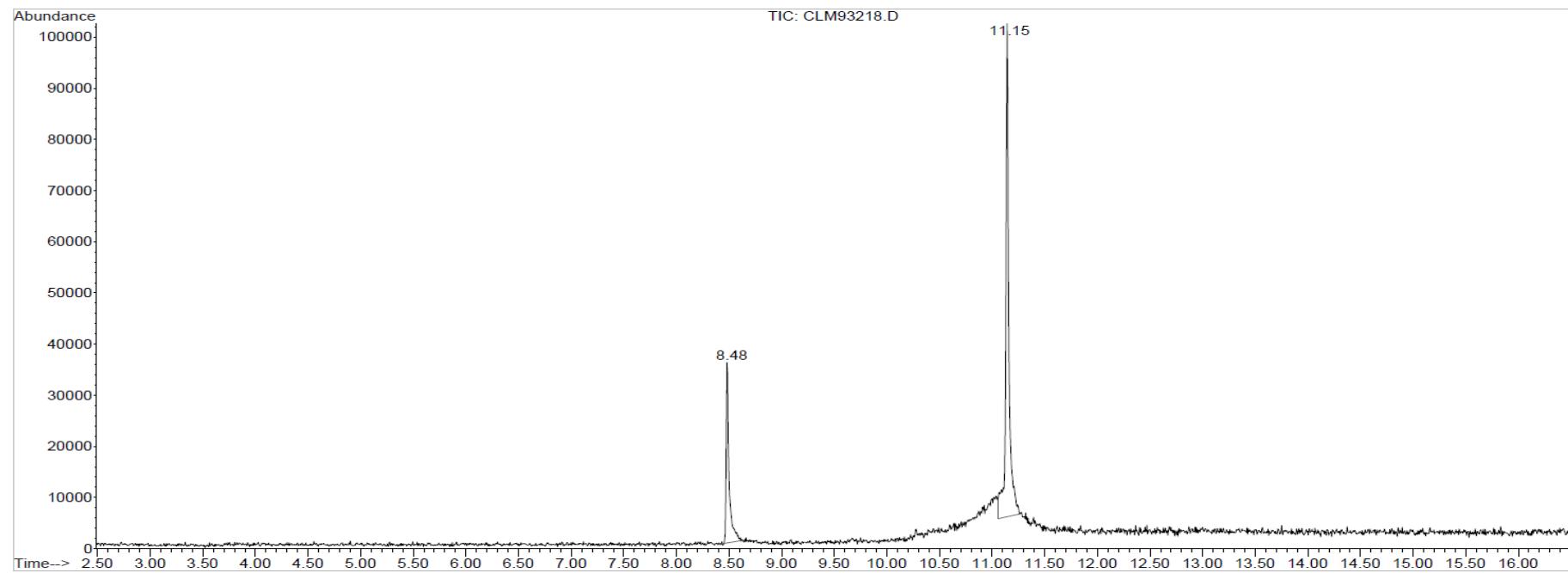
ischa-1ta\_no\_water\_11\_12\_2013

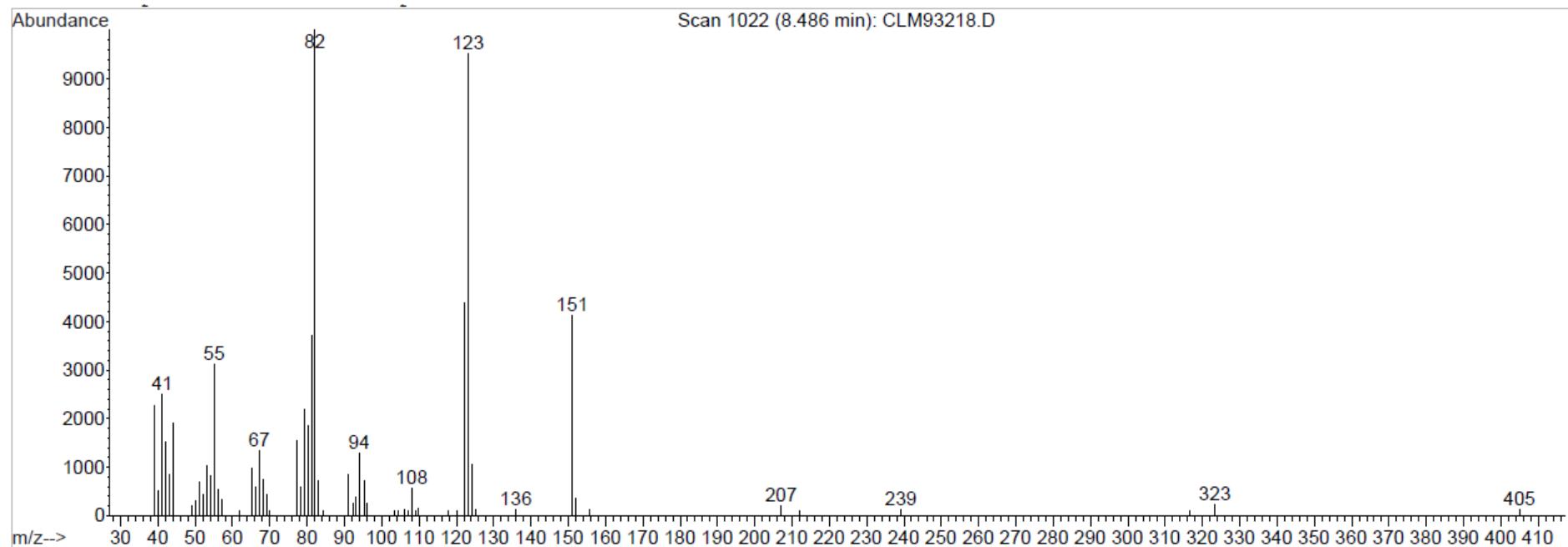


$^1\text{H}$ -NMR spectrum of **2** ( $\text{CD}_3\text{CN}$ , 500 MHz).



<sup>13</sup>C-NMR spectrum of **2** (CD<sub>3</sub>CN, 124.9 MHz).

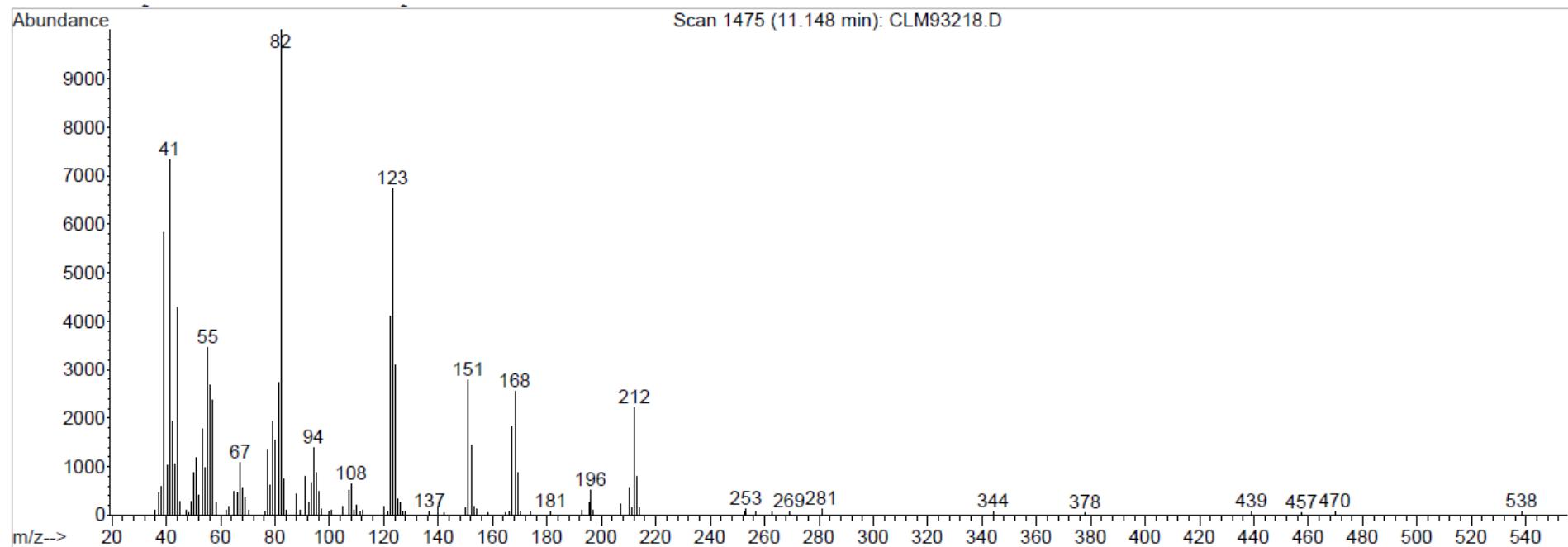




Data File: C:\MSDCHEM\1\DATA\G04\_15\CLM93218.D

Sample : CLM93218

Peak Number: 1 at 8.49 min Area: 668961 Area % 25.24



Data File: C:\MSDCHEM\1\DATA\G04\_15\CLM93218.D

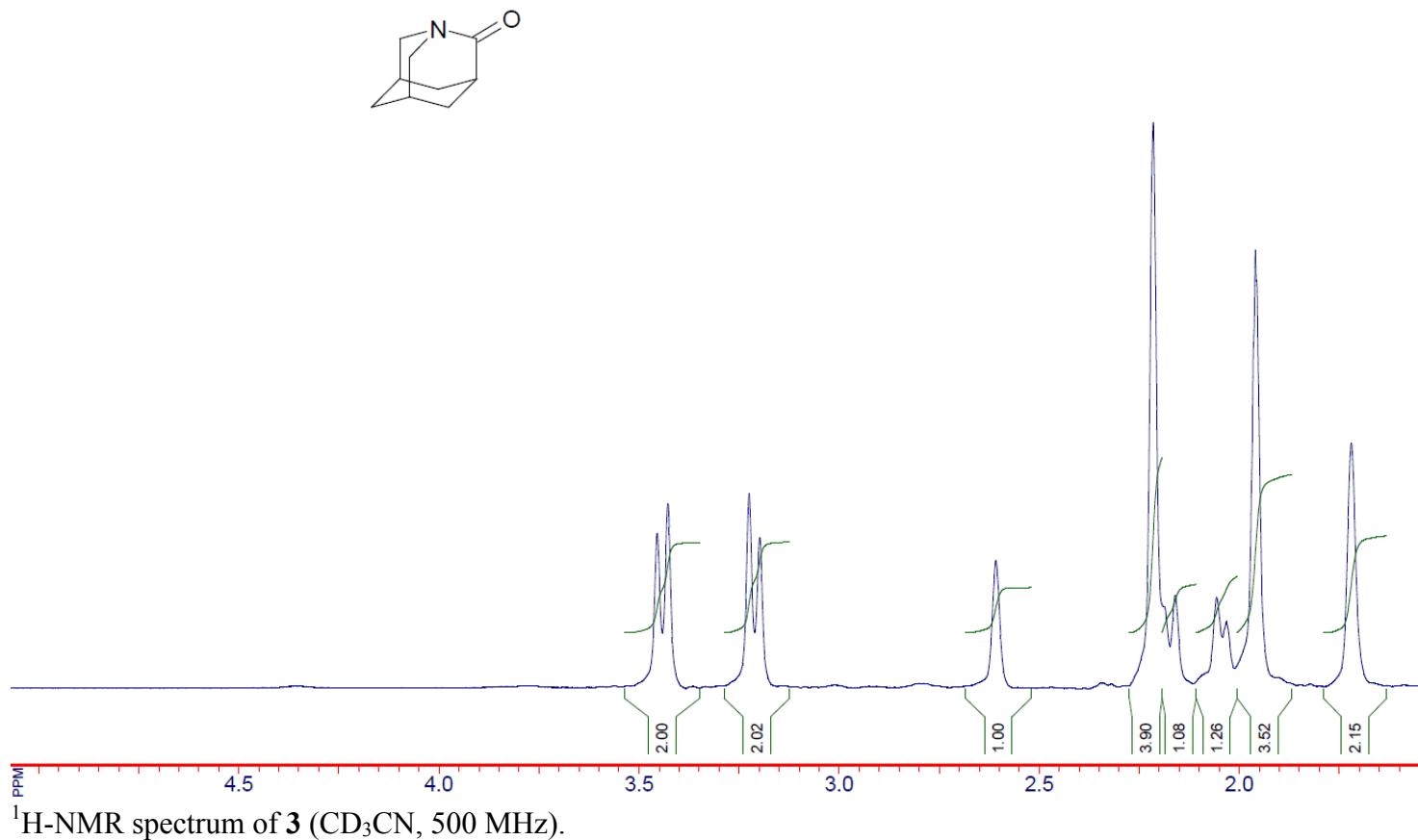
Sample : CLM93218

Peak Number: 2 at 11.15 min Area: 1981056 Area % 74.76

GS-MS trace for compound 8.

PPM

ischa-0310-01

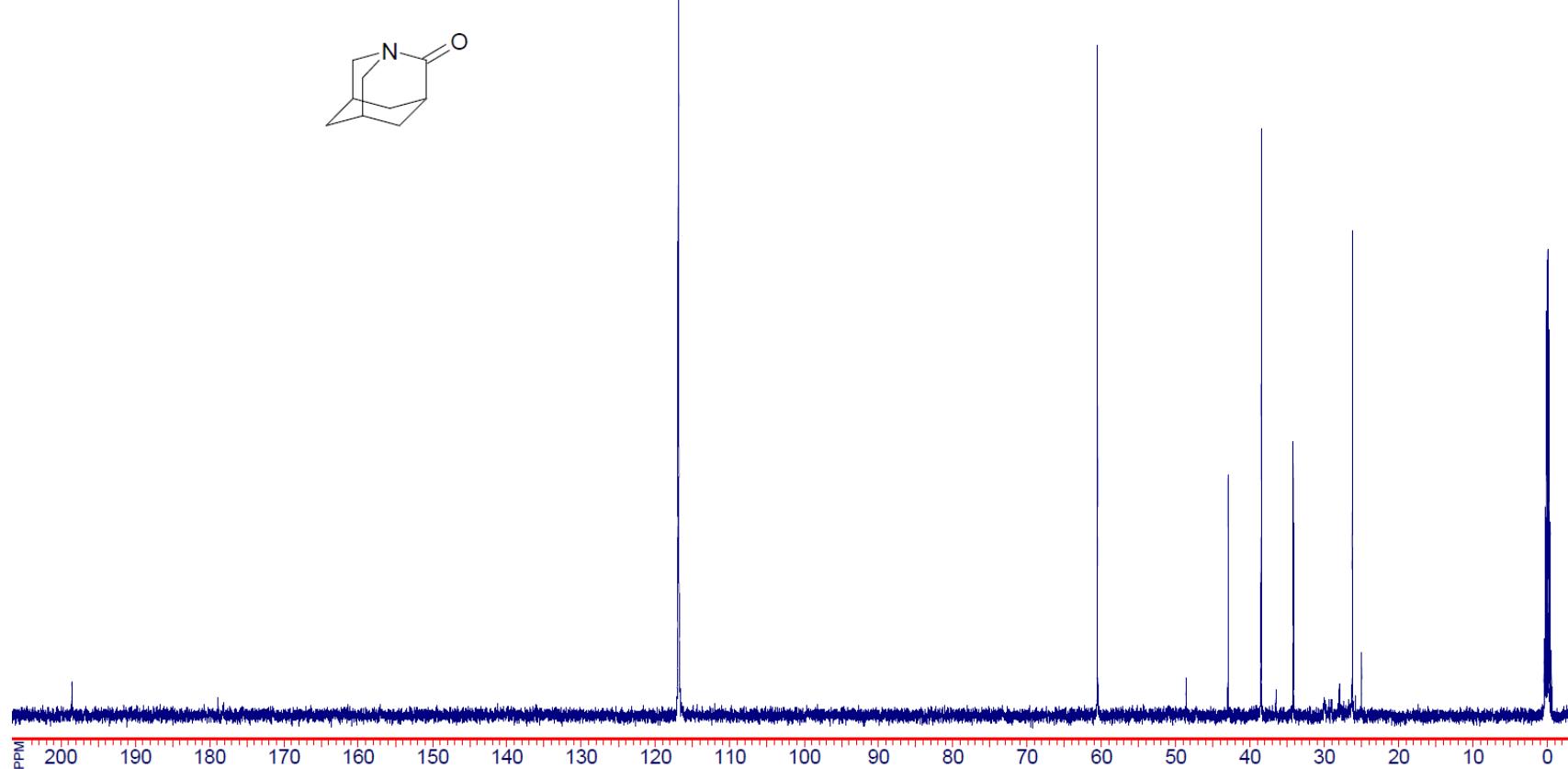
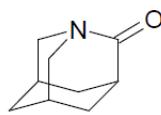


<sup>1</sup>H-NMR spectrum of 3 (CD<sub>3</sub>CN, 500 MHz).

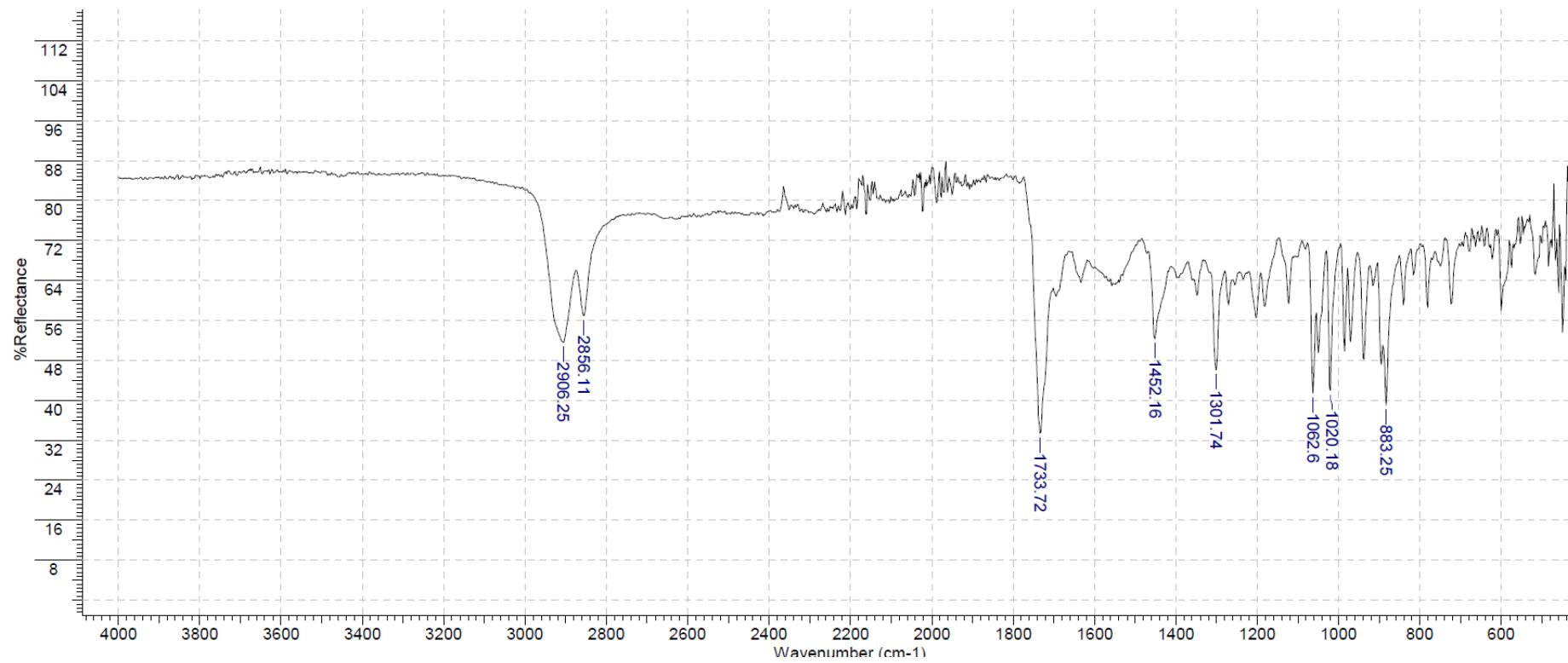
PPM

198.54

ischa-2910-01\_C13



$^{13}\text{C}$ -NMR spectrum of **3** ( $\text{CD}_3\text{CN}$ , 124.9 MHz).

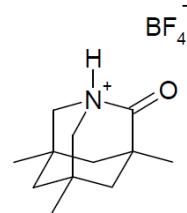


IR spectrum of **3** (Attenuated Total Reflectance (ATR) mode).

PPM

8.362

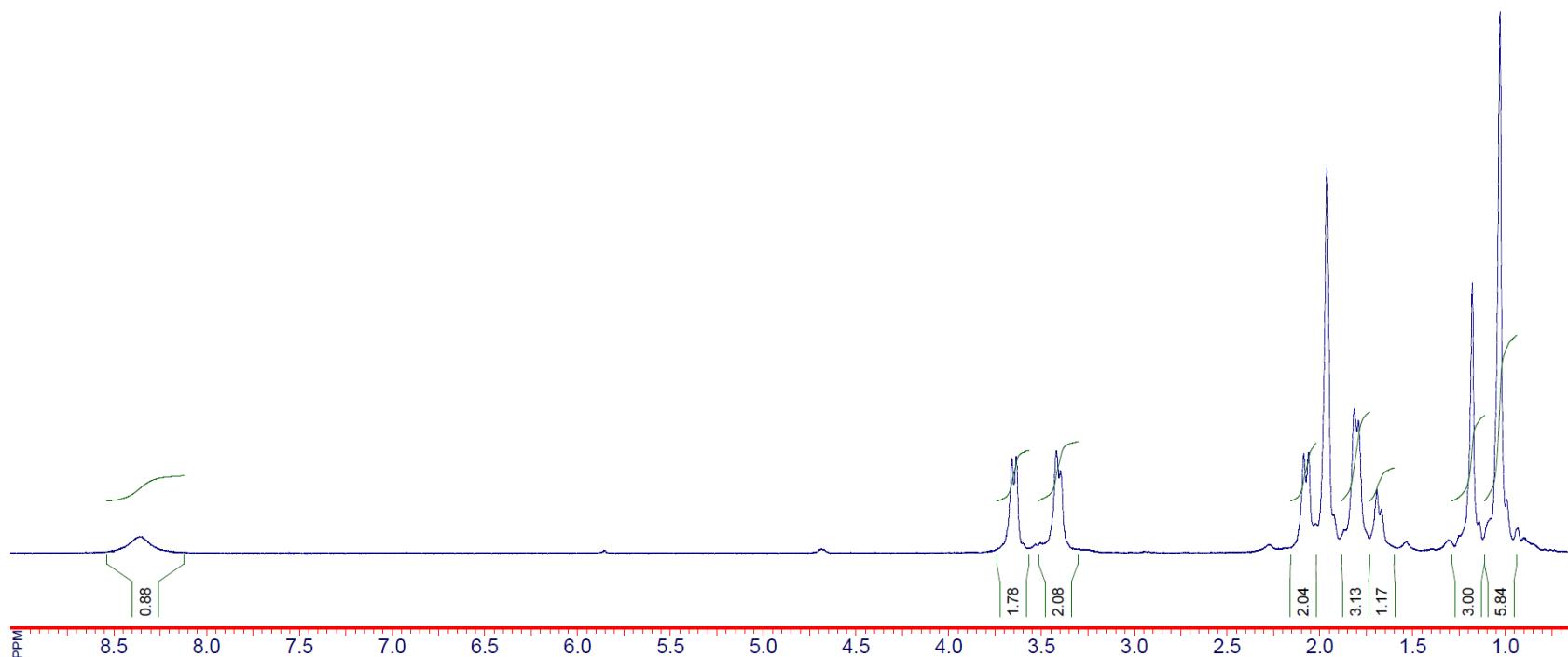
icsha-01



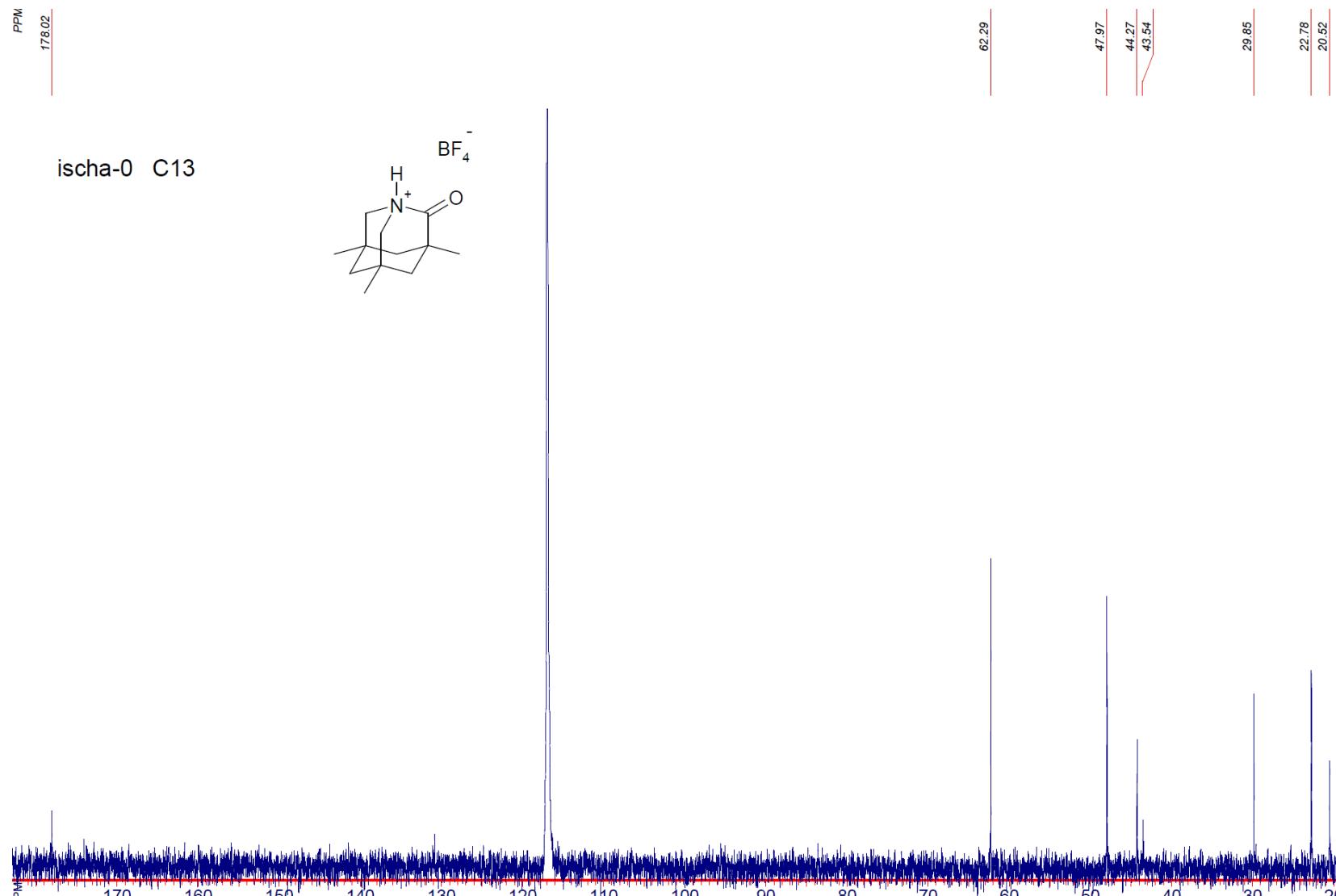
3.661  
3.637  
3.421  
3.397

2.087  
2.062  
1.963  
1.815  
1.793  
1.693  
1.667

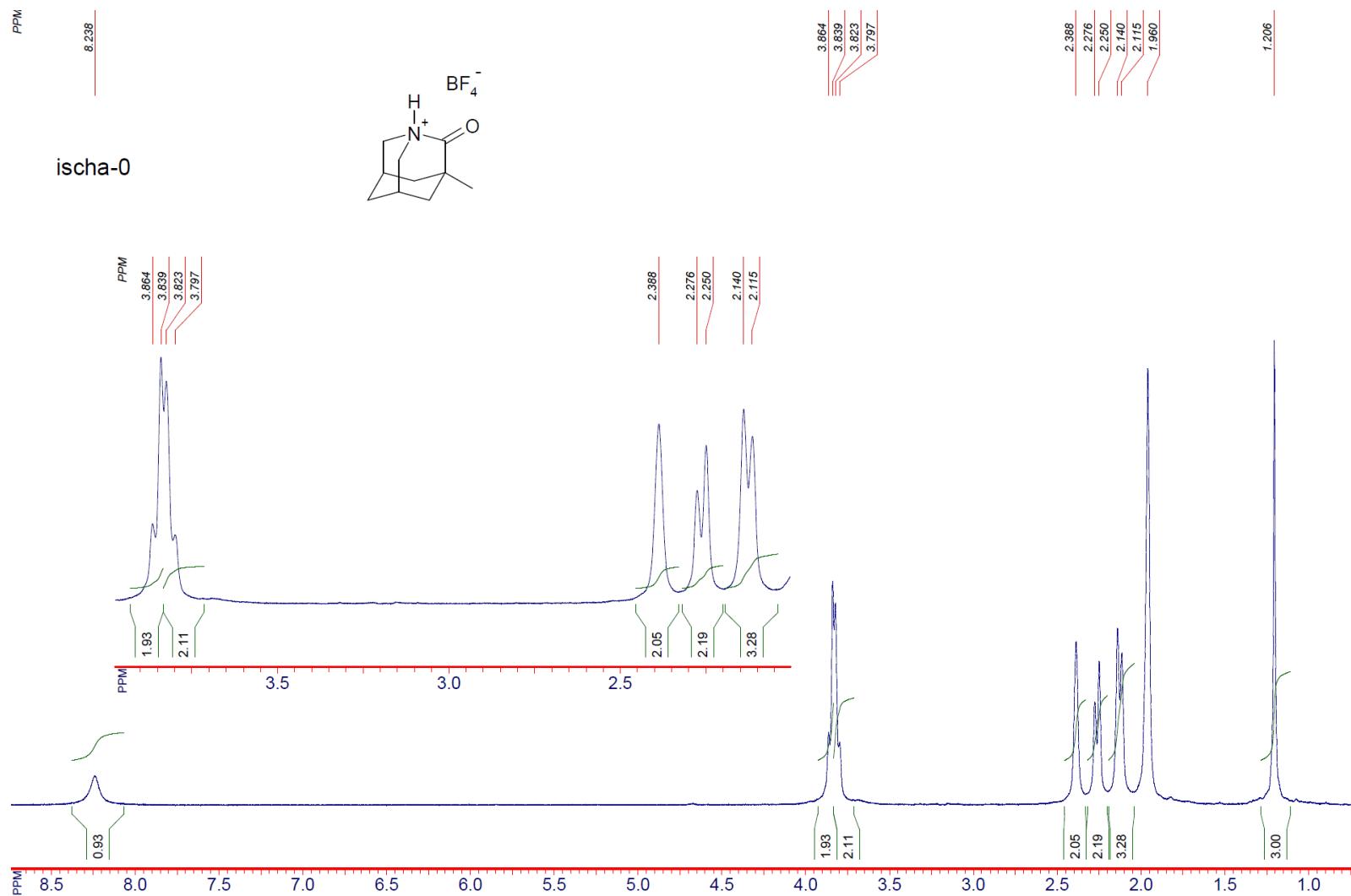
1.179  
1.030



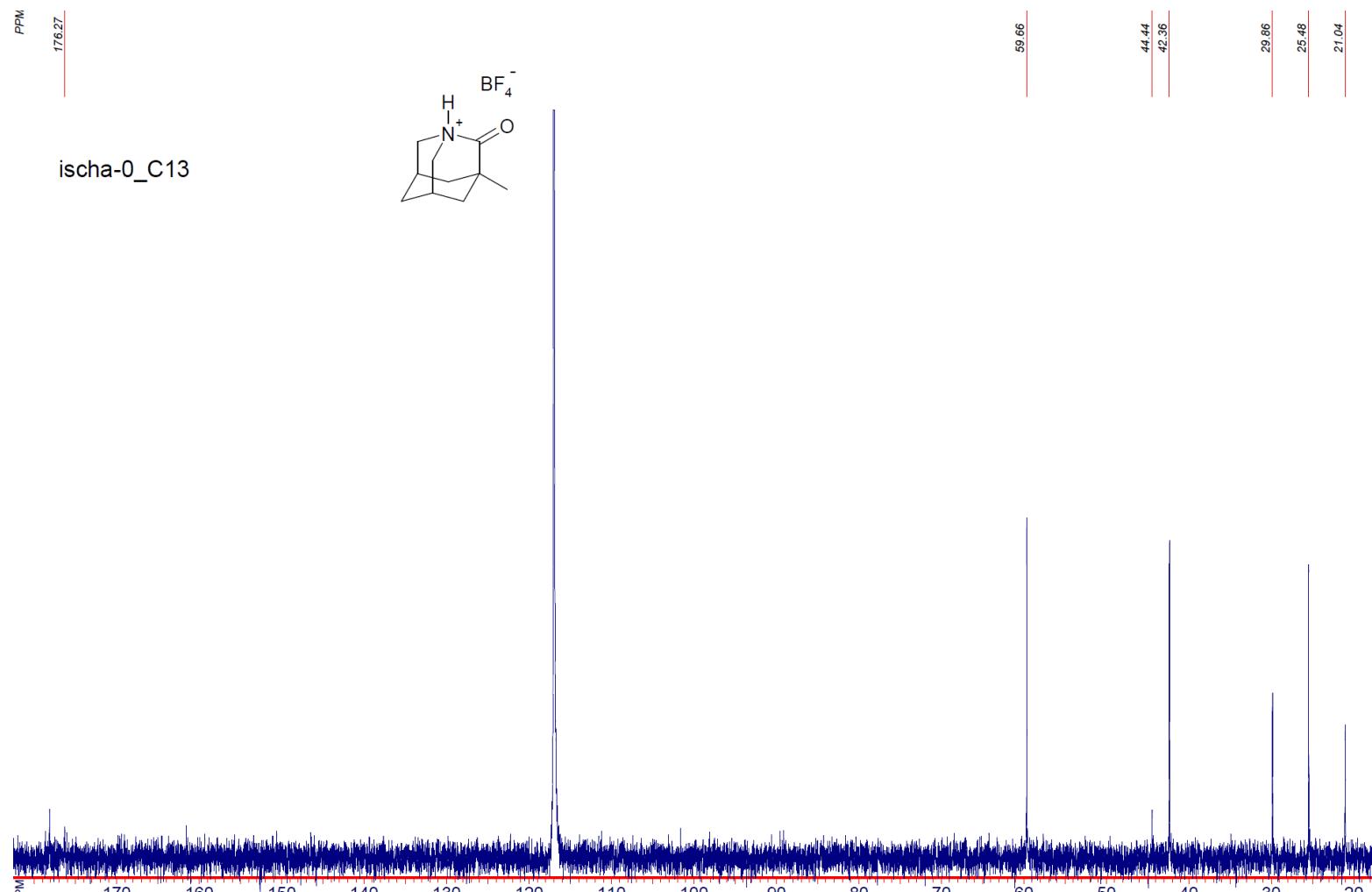
$^1\text{H}$ -NMR spectrum of **1** $\text{HBF}_4$  ( $\text{CD}_3\text{CN}$ , 500 MHz).



$^{13}\text{C}$ -NMR spectrum of **1** $\cdot\text{HBF}_4$  ( $\text{CD}_3\text{CN}$ , 124.9 MHz).



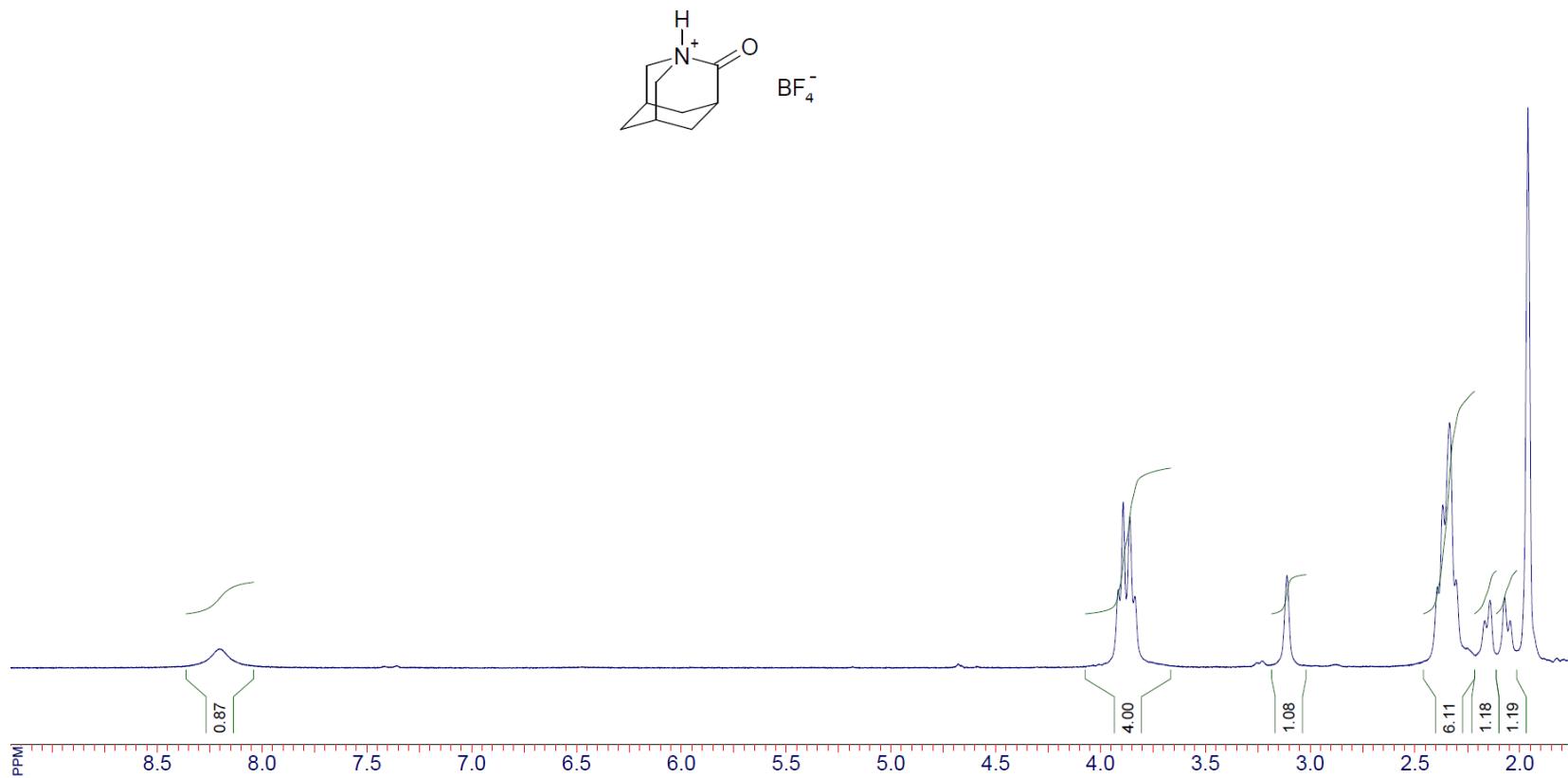
<sup>1</sup>H-NMR spectrum of **2**·HBF<sub>4</sub> (CD<sub>3</sub>CN, 500 MHz).



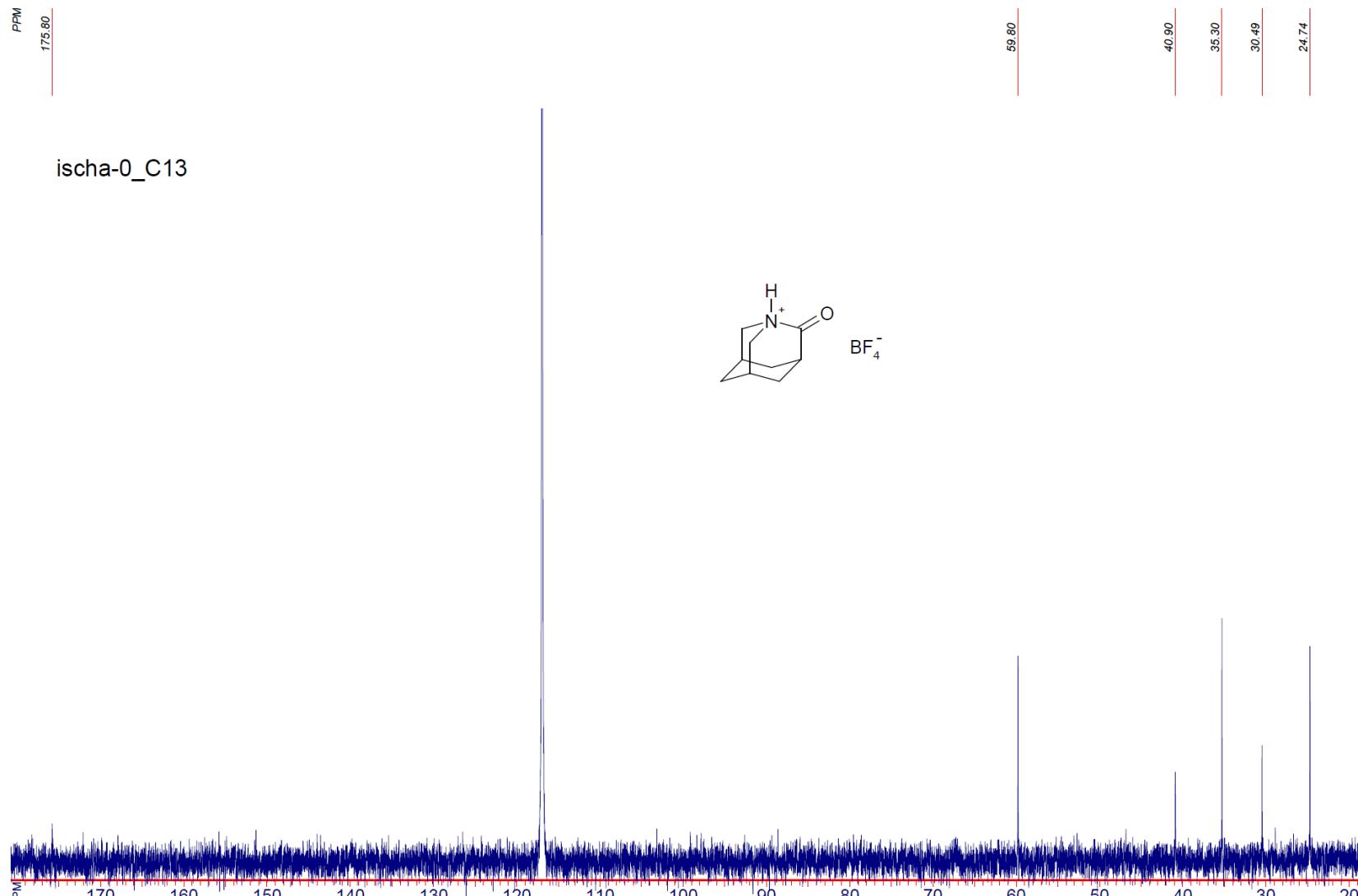
<sup>13</sup>C-NMR spectrum of **2**·HBF<sub>4</sub> (CD<sub>3</sub>CN, 124.9 MHz).

PPM

ischa-0



$^1\text{H}$ -NMR spectrum of **3** $\cdot\text{BF}_4^-$  ( $\text{CD}_3\text{CN}$ , 500 MHz).



<sup>13</sup>C-NMR spectrum of 3·BF<sub>4</sub> (CD<sub>3</sub>CN, 124.9 MHz).

PPM

7.517

4.438

3.943

3.620

3.133

3.108

3.035

2.980

2.959

2.838

2.668

2.334

1.953

1.766

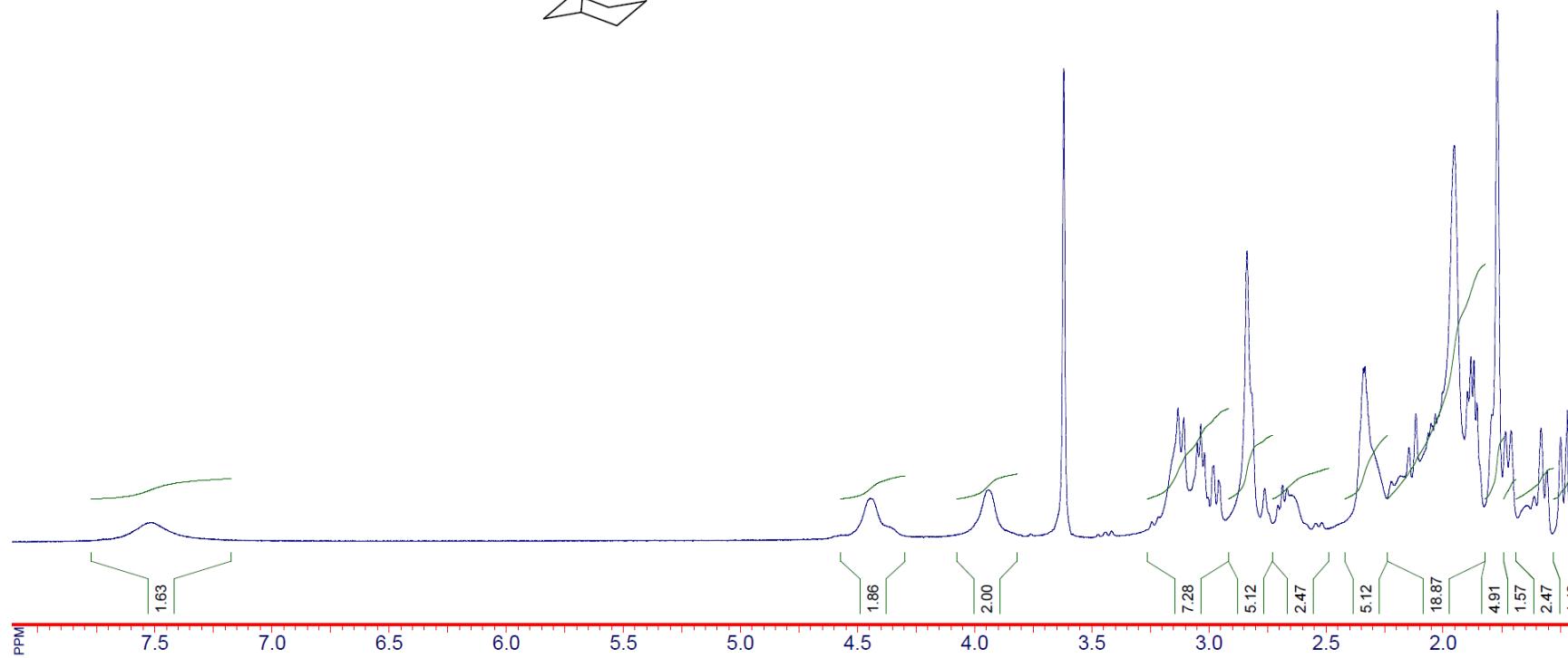
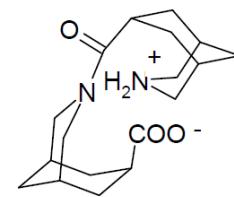
1.734

1.710

1.582

1.499

OTA\_ THF\_0\_6H<sub>2</sub>O\_75min



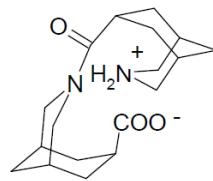
<sup>1</sup>H-NMR spectrum of the reaction mixture of **3** and 0.6 equiv. of water in THF-d<sub>8</sub> after 75 min of the reaction (500 MHz).

PPM

179.18

178.56

OTA\_ THF\_0\_6H2O\_75min\_13C



PPM

52.24

51.68

49.05

38.32

32.75

32.69

32.35

32.00

31.34

29.69

29.14

27.98

27.17

52.24

51.68

49.05

38.32

32.75

32.59

32.35

32.00

31.34

29.69

29.14

PPM

170

160

150

140

130

120

110

100

90

80

70

60

50

40

30

20

10

0

$^{13}\text{C}$ -NMR spectrum of the reaction mixture of **3** and 0.6 equiv. of water in  $\text{THF-d}_8$  after 75 min of the reaction (124.9 MHz).