

ESI(P),C4-1,20160315

Analysis Info

Analysis Name D:\Data\ESI\2016\2016-03\0315\C4-1_000001.d

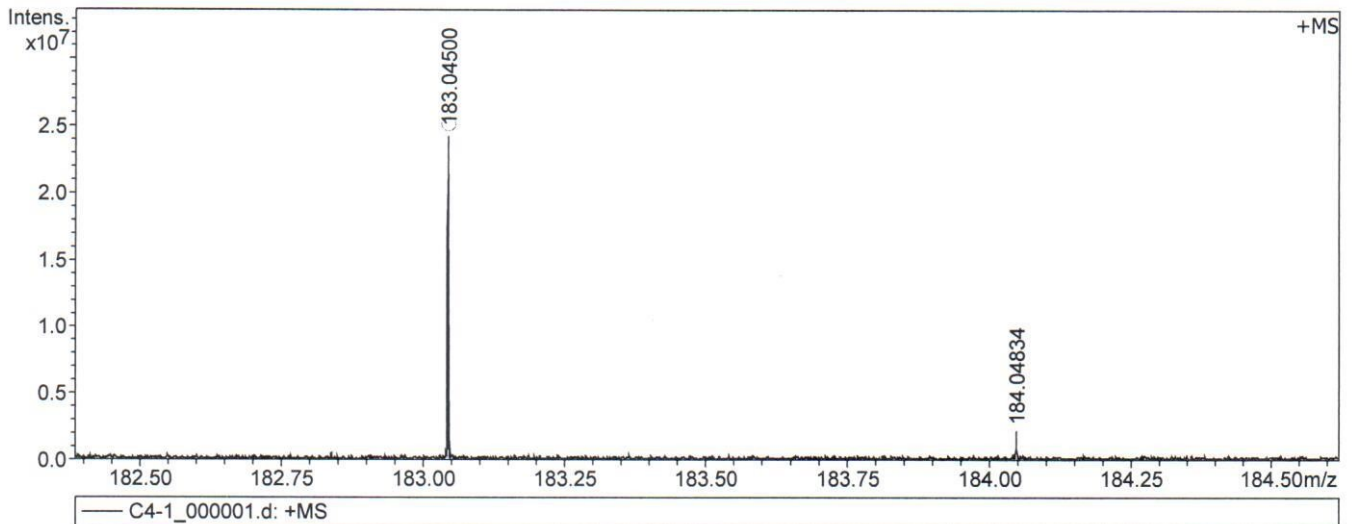
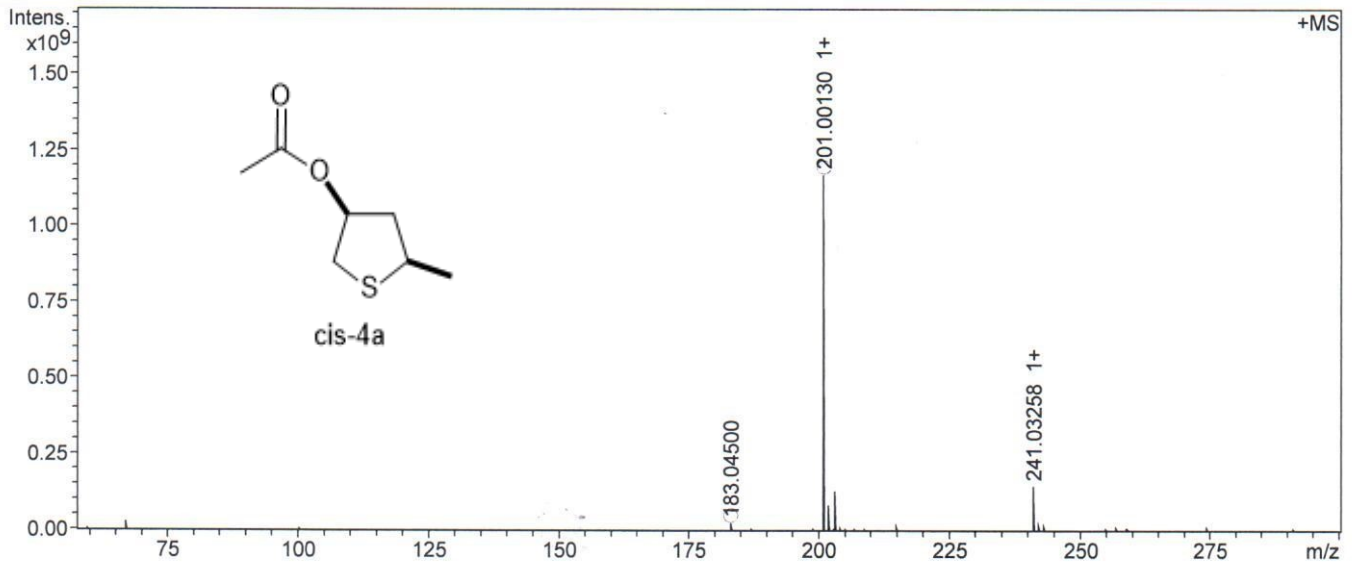
Acquisition Date 3/15/2016 10:39:21 AM

Sample Name C4-1

Instrument solariX

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	8	Calibration Date	Thu Mar 10 09:43:56
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	2046576
Broadband Low Mass	57.7 m/z	Source Accumulation	0.001 sec	Data Processing Size	2097152
Broadband High Mass	300.0 m/z	Ion Accumulation Time	0.100 sec	Apodization	Sine-Bell Multiplication



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
183.044998	1	C7H12NaO2S	100.00	183.045021	-0.1	-0.0	26.3	1.5	even	ok
201.001305	1	C4H5N6S2	100.00	201.001163	0.7	-1.4	10.9	5.5	even	ok
	1	C6H10NaO2S2	100.00	201.001442	-0.7	0.8	9.3	1.5	even	ok

ESI(P),C4-2,20160315

Analysis Info

Analysis Name D:\Data\ESI\2016\2016-03\0315\C4-2_000002.d

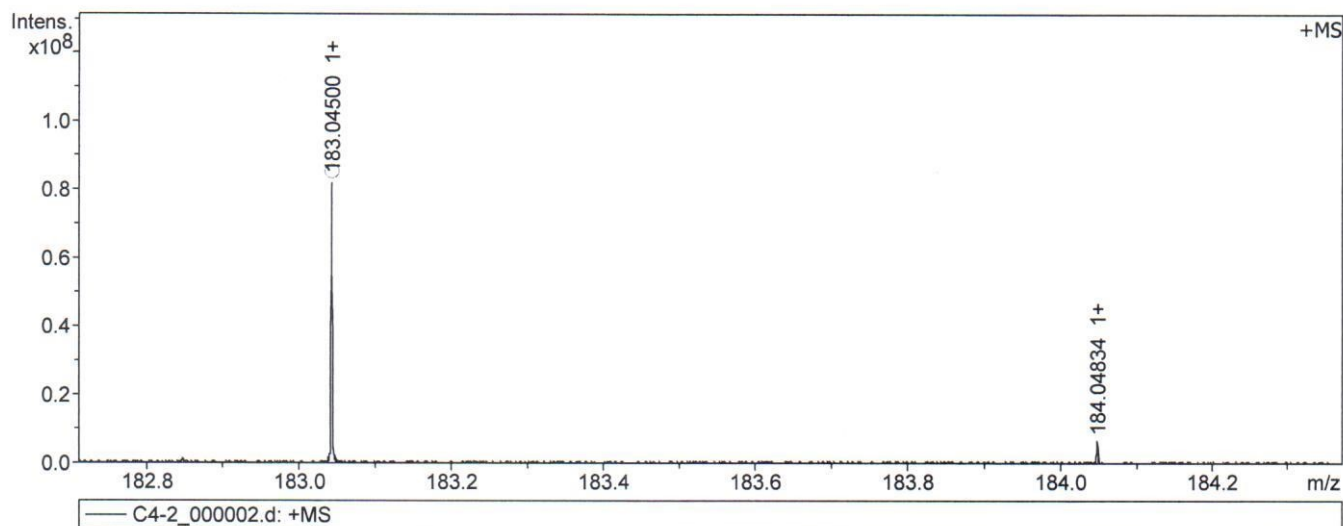
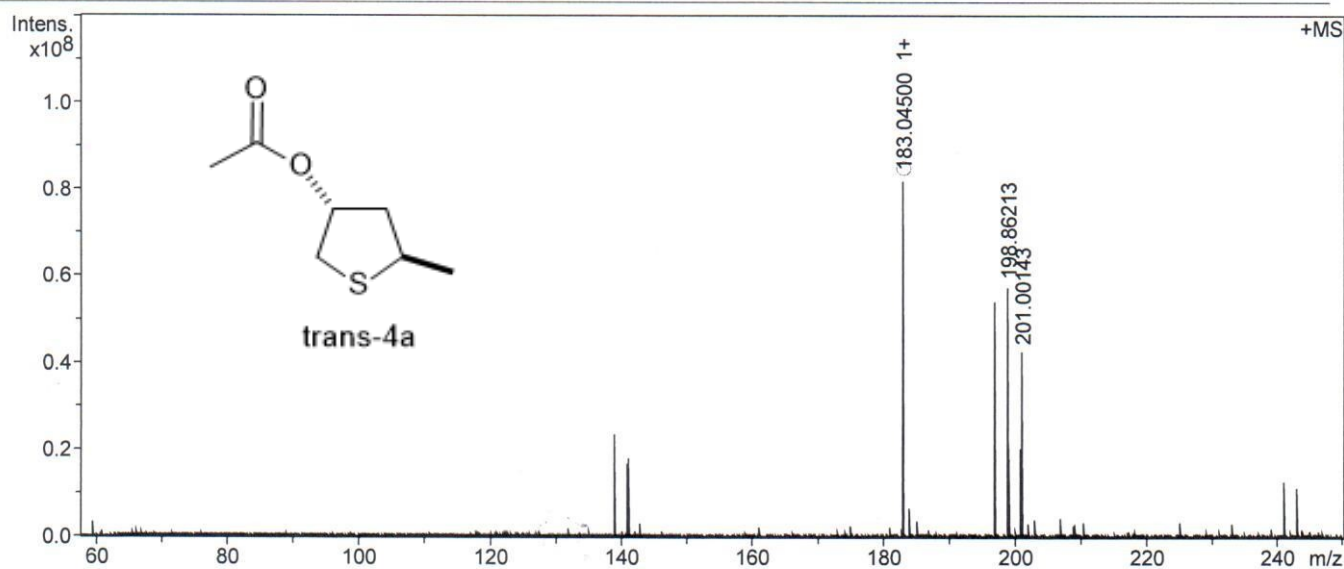
Acquisition Date 3/15/2016 10:56:48 AM

Sample Name C4-2

Instrument solariX

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	20	Calibration Date	Thu Mar 10 09:43:56
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	2046576
Broadband Low Mass	57.7 m/z	Source Accumulation	0.001 sec	Data Processing Size	2097152
Broadband High Mass	250.0 m/z	Ion Accumulation Time	0.200 sec	Apodization	Sine-Bell Multiplication



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
183.045004	1	C7H12NaO2S	100.00	183.045021	-0.1	-0.0	26.2	1.5	even	ok

ESI(P),d4-1,20160315

Analysis Info

Analysis Name D:\Data\ESI\2016\2016-03\0315\d4-1_000001.d

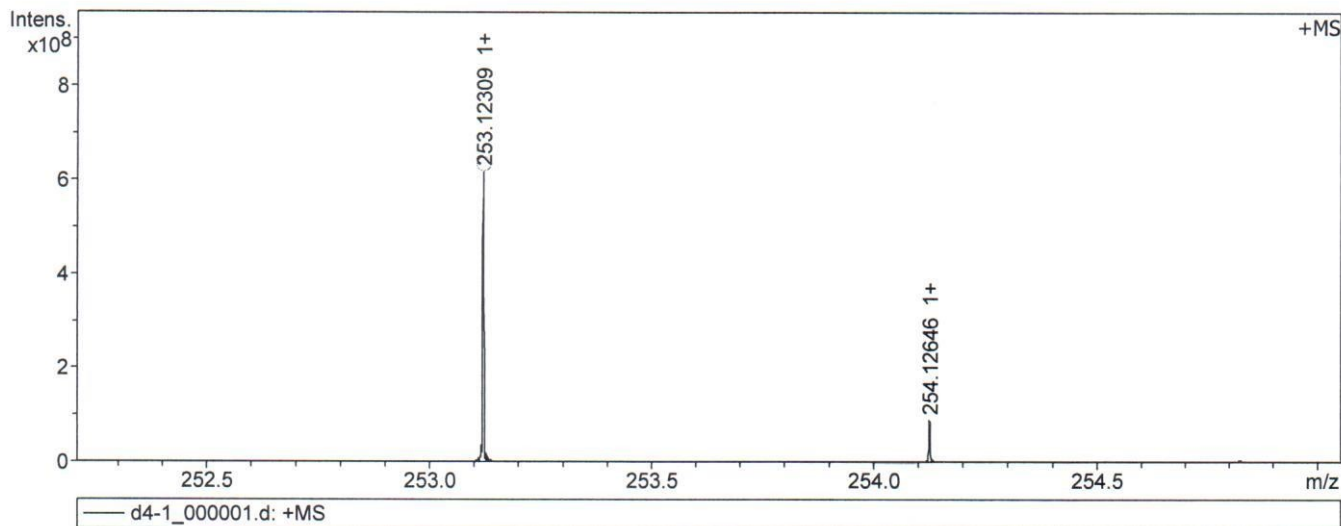
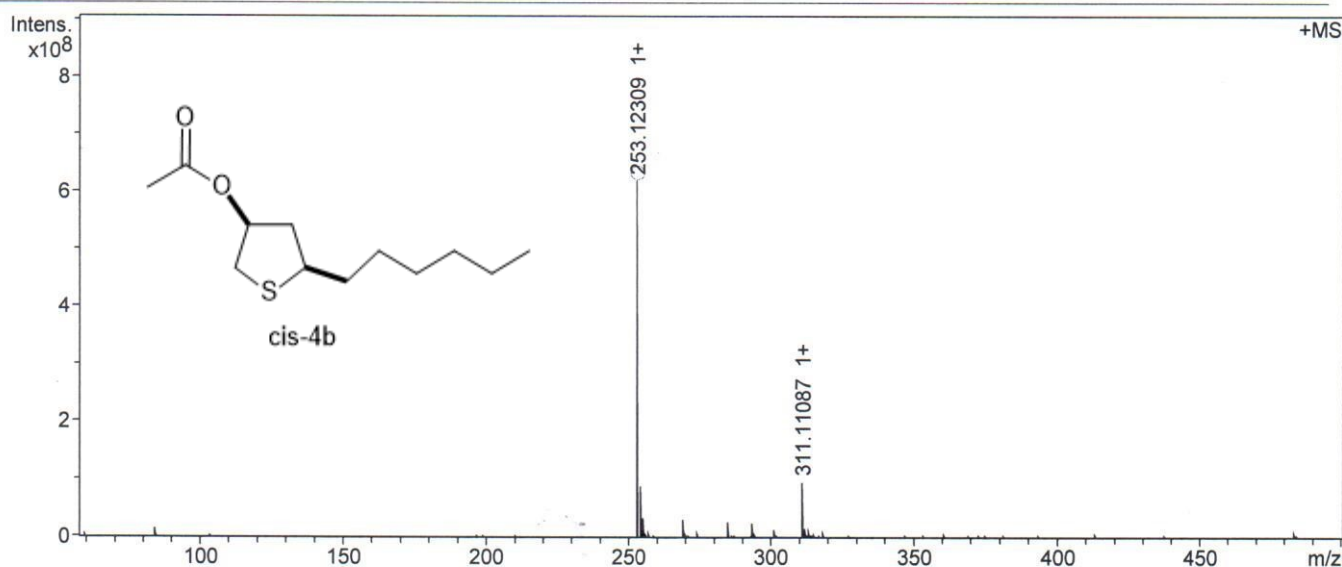
Acquisition Date 3/15/2016 11:10:40 AM

Sample Name d4-1

Instrument solariX

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	4	Calibration Date	Thu Mar 10 09:43:56
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	2048576
Broadband Low Mass	57.7 m/z	Source Accumulation	0.001 sec	Data Processing Size	2097152
Broadband High Mass	500.0 m/z	Ion Accumulation Time	0.100 sec	Apodization	Sine-Bell Multiplication



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
253.123087	1	C ₁₂ H ₂₂ NaO ₂ S	100.00	253.123272	-0.7	0.6	27.0	1.5	even	ok

ESI(P),d4-2,20160315

Analysis Info

Analysis Name D:\Data\ESI\2016\2016-03\0315\d4-2_000002.d

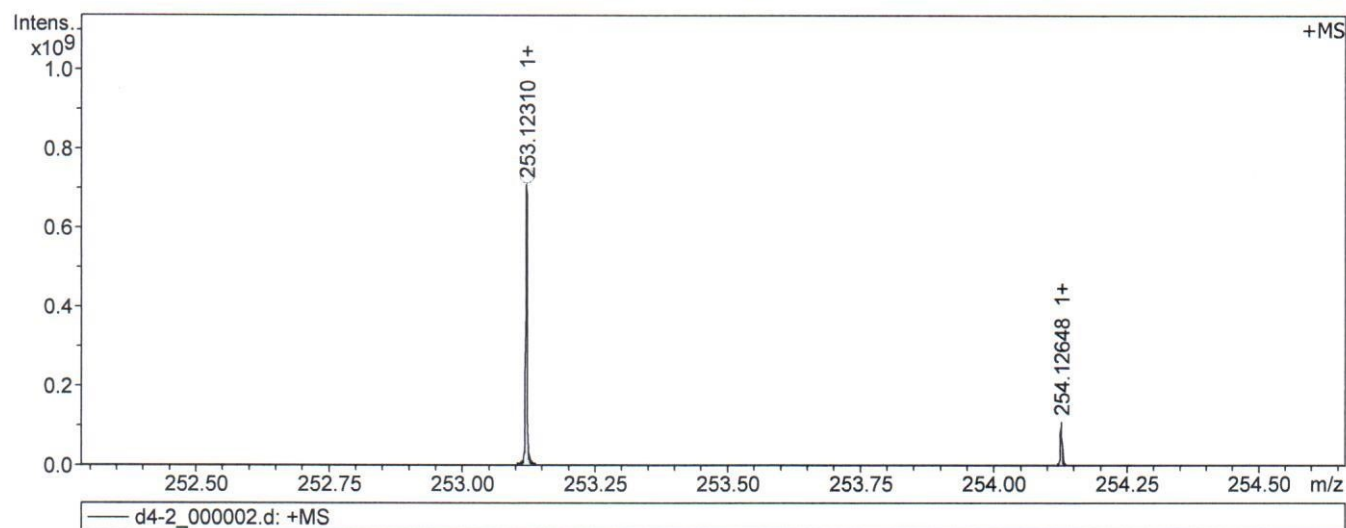
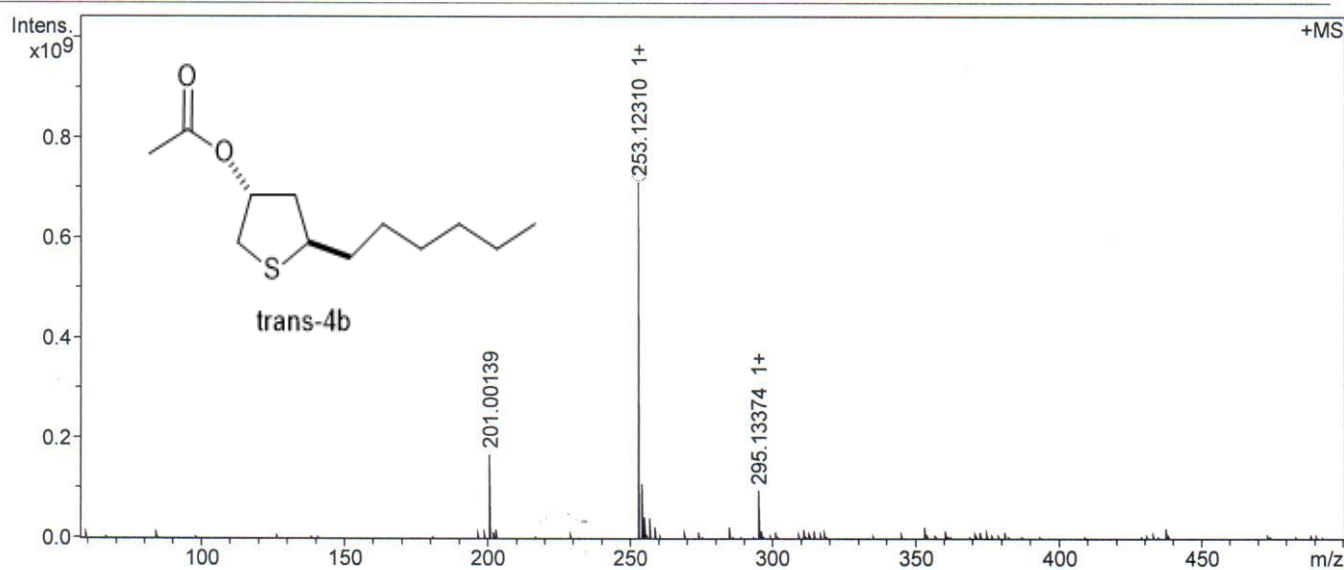
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Sample Name d4-2

Instrument solariX

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	10	Calibration Date	Thu Mar 10 09:43:56
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	2046576
Broadband Low Mass	57.7 m/z	Source Accumulation	0.001 sec	Data Processing Size	2097152
Broadband High Mass	500.0 m/z	Ion Accumulation Time	0.100 sec	Apodization	Sine-Bell Multiplication



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
253.123104	1	C ₁₂ H ₂₂ NaO ₂ S	100.00	253.123272	-0.7	0.6	27.9	1.5	even	ok

ESI(P),F4-1,20160804

Analysis Info

Analysis Name D:\Data\ESI\2016\2016-08\0804\F4-1_000002.d

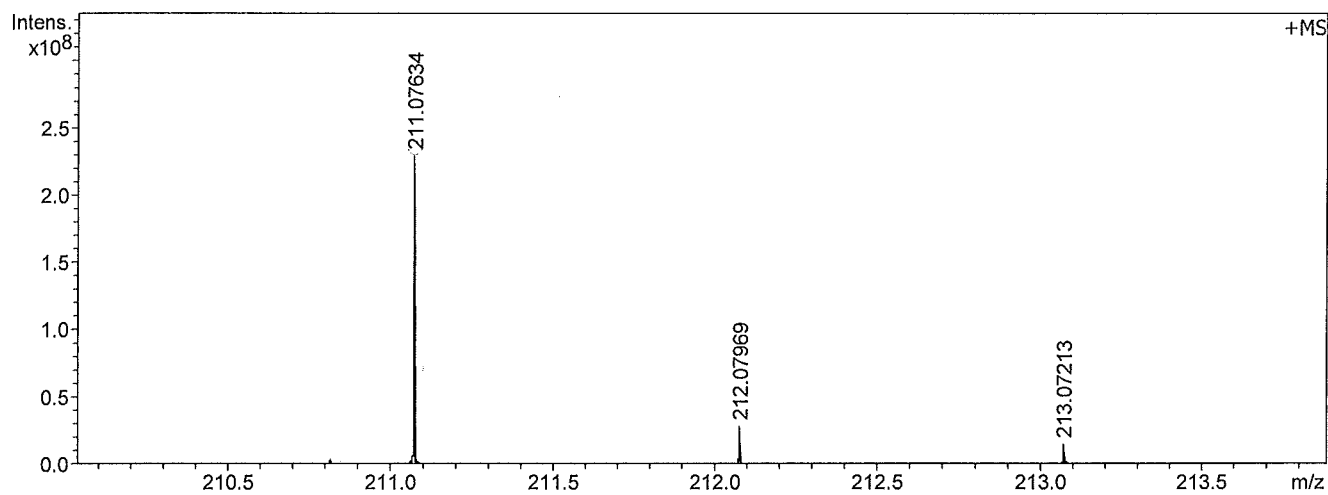
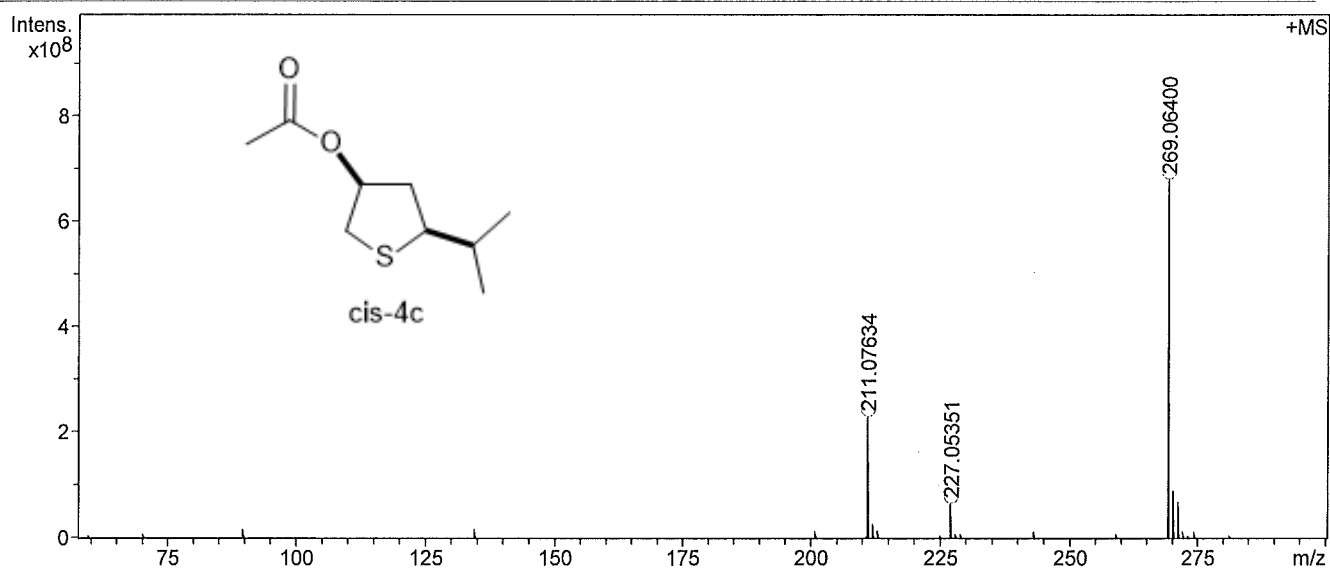
Acquisition Date 8/4/2016 9:20:11 AM

Sample Name F4-1

Instrument solarix

Acquisition Parameter

Polarity Positive Acquired Scans 4
Broadband Low Mass 57.7 m/z Broadband High Mass 300.0 m/z



F4-1_000002.d: +MS

Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
211.076337	1	C ₉ H ₁₆ NaO ₂ S	100.00	211.076321	0.1	-0.2	26.0	1.5	even	ok
227.053507	1	C ₉ H ₁₆ NaOS ₂	100.00	227.053478	0.1	-0.1	9.2	1.5	even	ok
269.064004	1	C ₁₁ H ₁₈ NaO ₂ S ₂	100.00	269.064043	-0.1	0.4	2.4	2.5	even	ok

ESI(P),F4-2,20160804

Analysis Info

Analysis Name D:\Data\ESI\2016\2016-08\0804\F4-2_000001.d

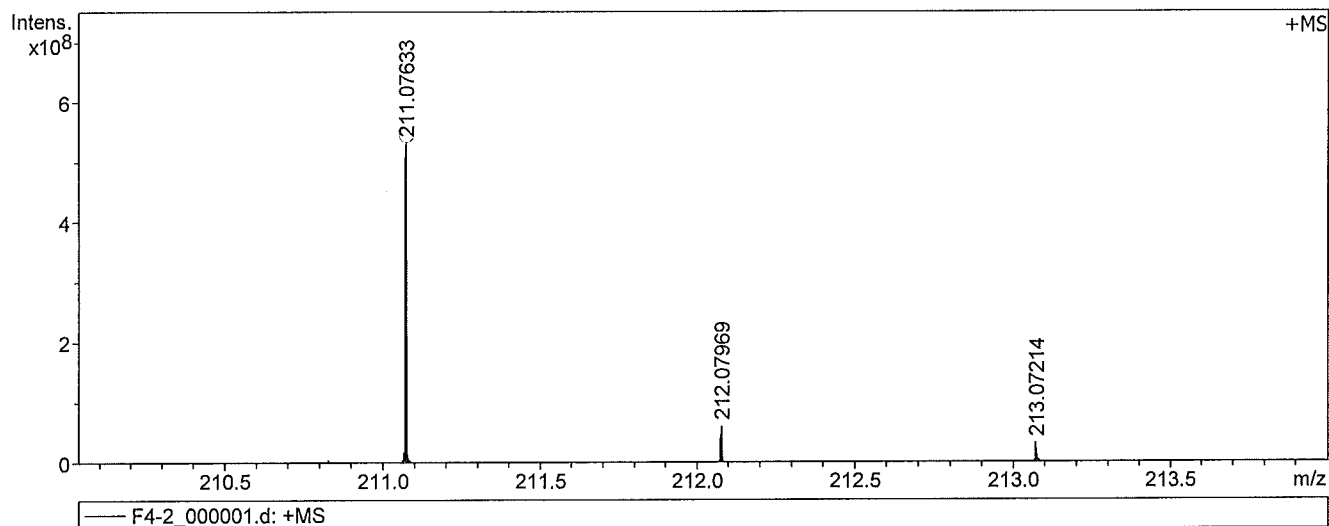
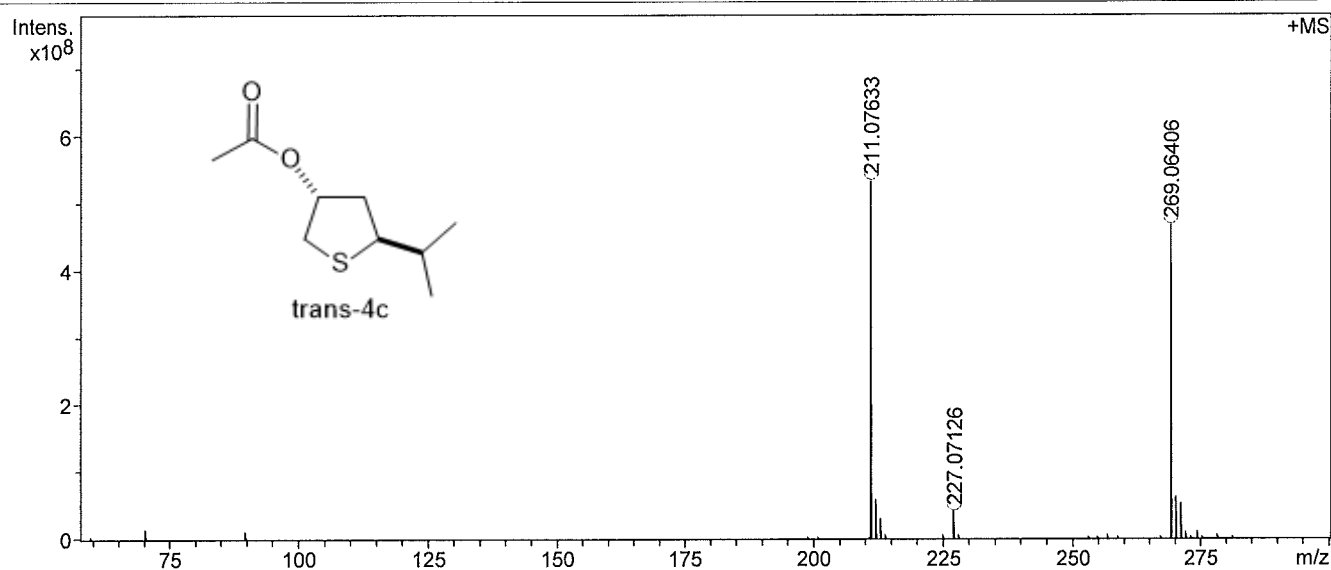
Acquisition Date 8/4/2016 9:33:06 AM

Sample Name F4-2

Instrument solarix

Acquisition Parameter

Polarity Positive
Acquired Scans 4
Broadband Low Mass 57.7 m/z
Broadband High Mass 300.0 m/z



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
211.076328	1	C ₉ H ₁₆ NaO ₂ S	100.00	211.076321	-0.0	-0.1	25.1	1.5	even	ok
227.071261	1	C ₉ H ₁₆ NaO ₃ S	100.00	227.071236	0.1	-0.2	27.0	1.5	even	ok
269.064062	1	C ₁₁ H ₁₈ NaO ₂ S ₂	100.00	269.064043	-0.1	0.2	6.3	2.5	even	ok

ESI(P),H4-1,20160804

Analysis Info

Analysis Name D:\Data\ESI\2016\2016-08\0804\H4-1_000001.d

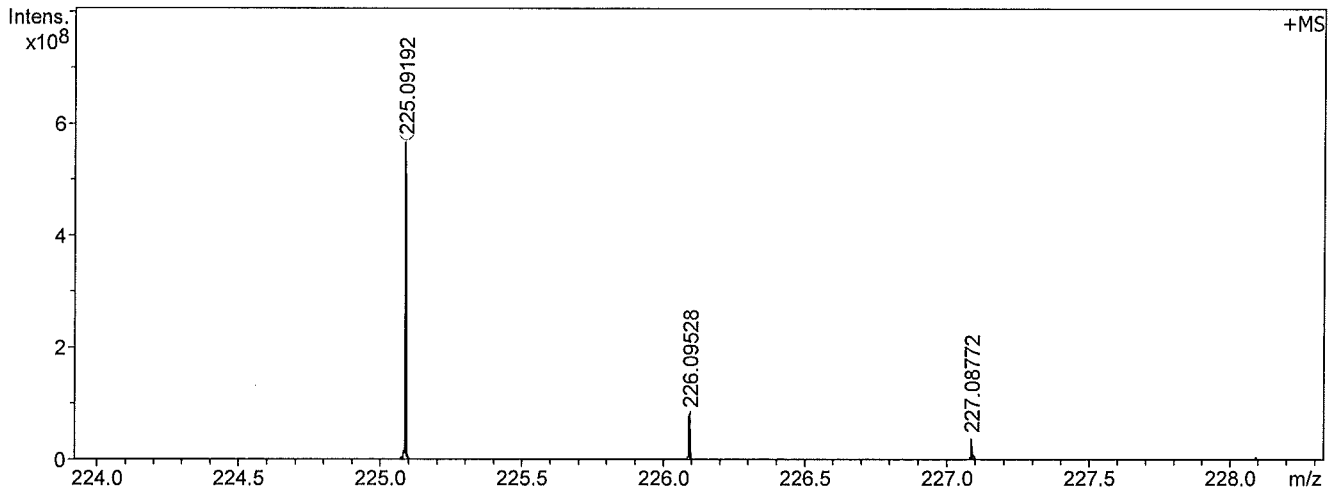
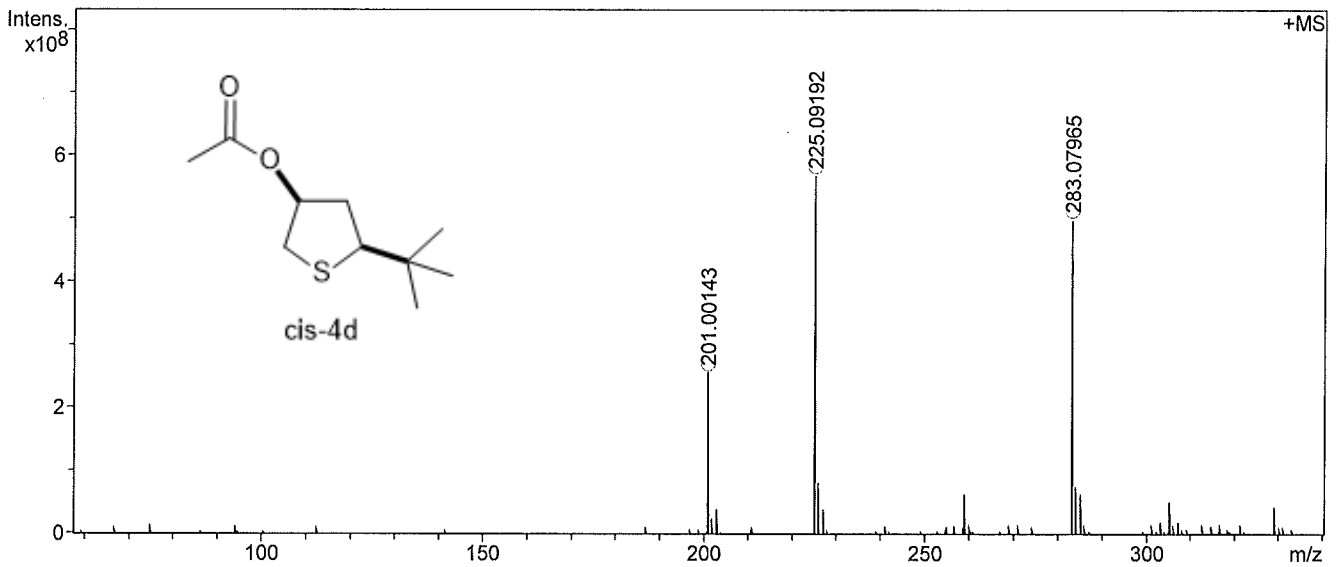
Acquisition Date 8/4/2016 10:08:36 AM

Sample Name H4-1

Instrument solarix

Acquisition Parameter

Polarity Positive
Acquired Scans 10
Broadband Low Mass 57.7 m/z
Broadband High Mass 340.0 m/z



H4-1_000001.d: +MS

Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
201.001428	1	C6H10NaO2S2	100.00	201.001442	0.1	0.2	29.7	1.5	even	ok
225.091918	1	C10H18NaO2S	100.00	225.091972	-0.2	0.6	14.0	1.5	even	ok
283.079652	1	C12H20NaO2S2	100.00	283.079693	0.1	0.5	11.5	2.5	even	ok

ESI(P),H4-2,20160804

Analysis Info

Analysis Name D:\Data\ESI\2016\2016-08\0804\H4-2_000001.d

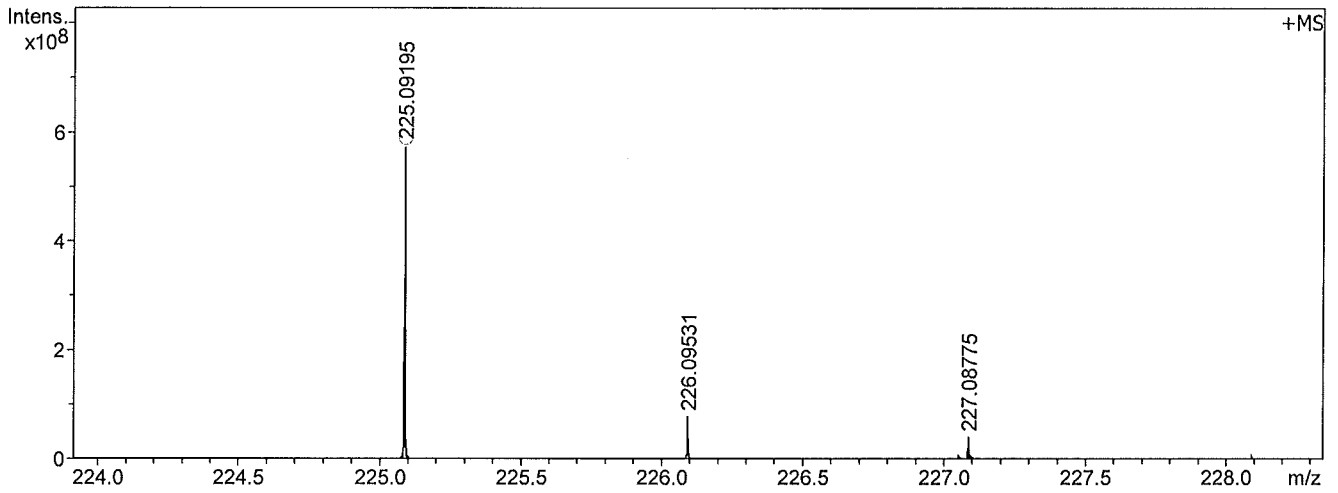
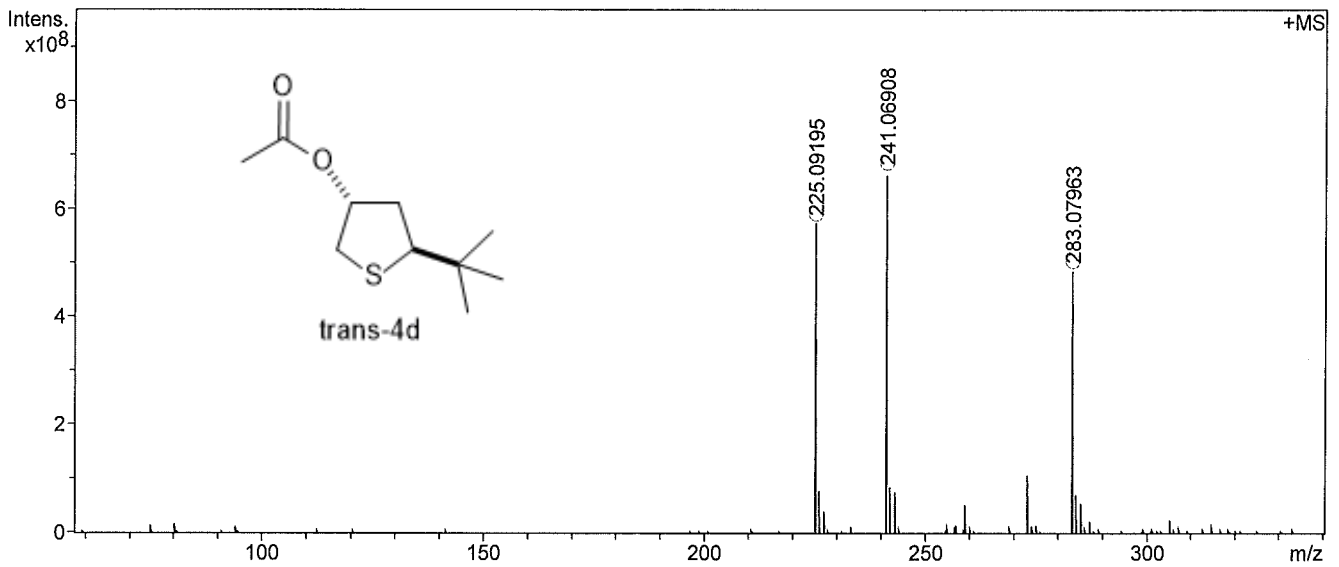
Acquisition Date 8/4/2016 10:20:11 AM

Sample Name H4-2

Instrument solarix

Acquisition Parameter

Polarity Positive Acquired Scans 10
Broadband Low Mass 57.7 m/z Broadband High Mass 340.0 m/z



H4-2_000001.d: +MS

Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
225.091949	1	C ₁₀ H ₁₈ NaO ₂ S	100.00	225.091972	0.1	-0.0	26.6	1.5	even	ok
241.069077	1	C ₁₀ H ₁₈ NaOS ₂	100.00	241.069128	0.2	0.4	7.2	1.5	even	ok
283.079635	1	C ₁₂ H ₂₀ NaO ₂ S ₂	100.00	283.079693	0.2	0.5	5.7	2.5	even	ok

ESI(P),B4-2,20160315

Analysis Info

Analysis Name D:\Data\ESI\2016\2016-03\0315\B4-2_000002.d

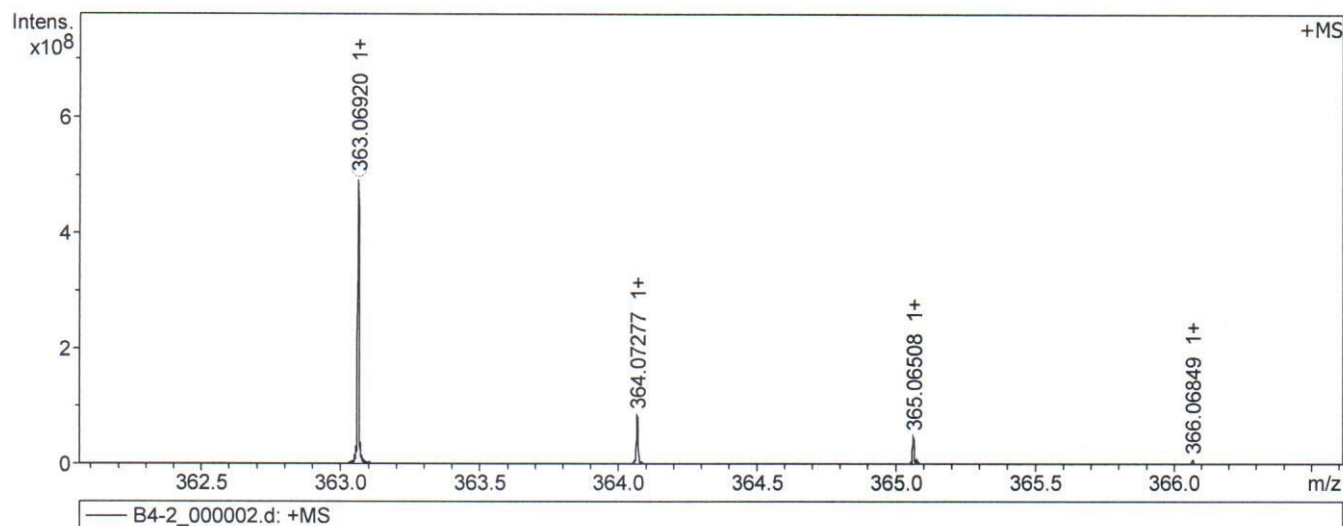
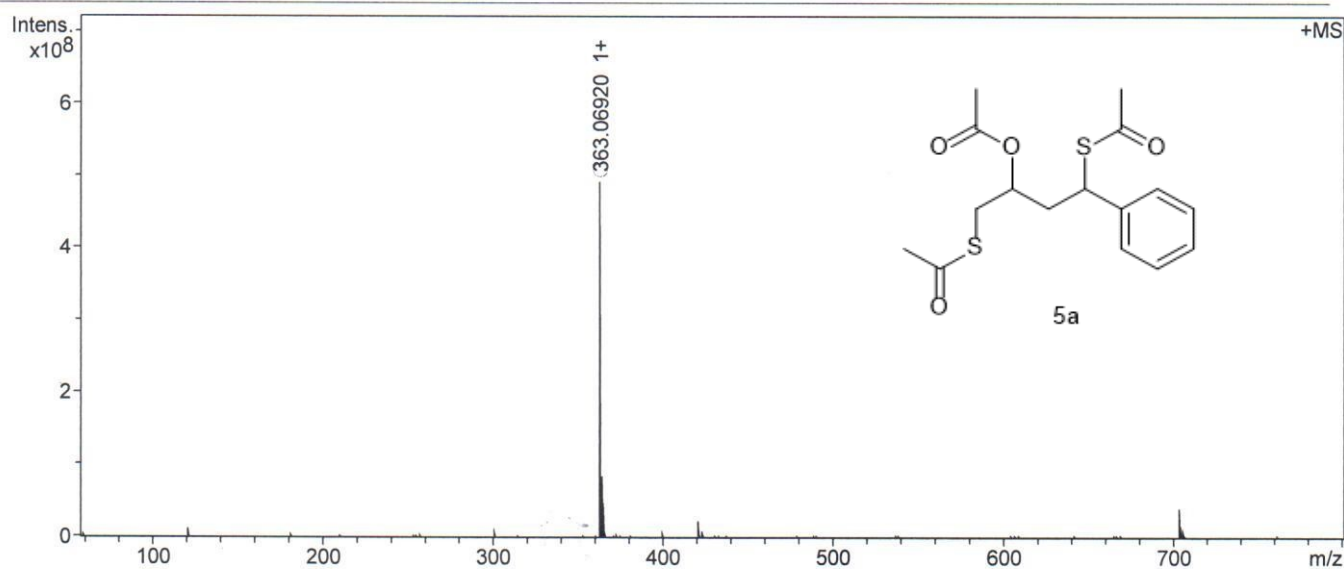
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Sample Name B4-2

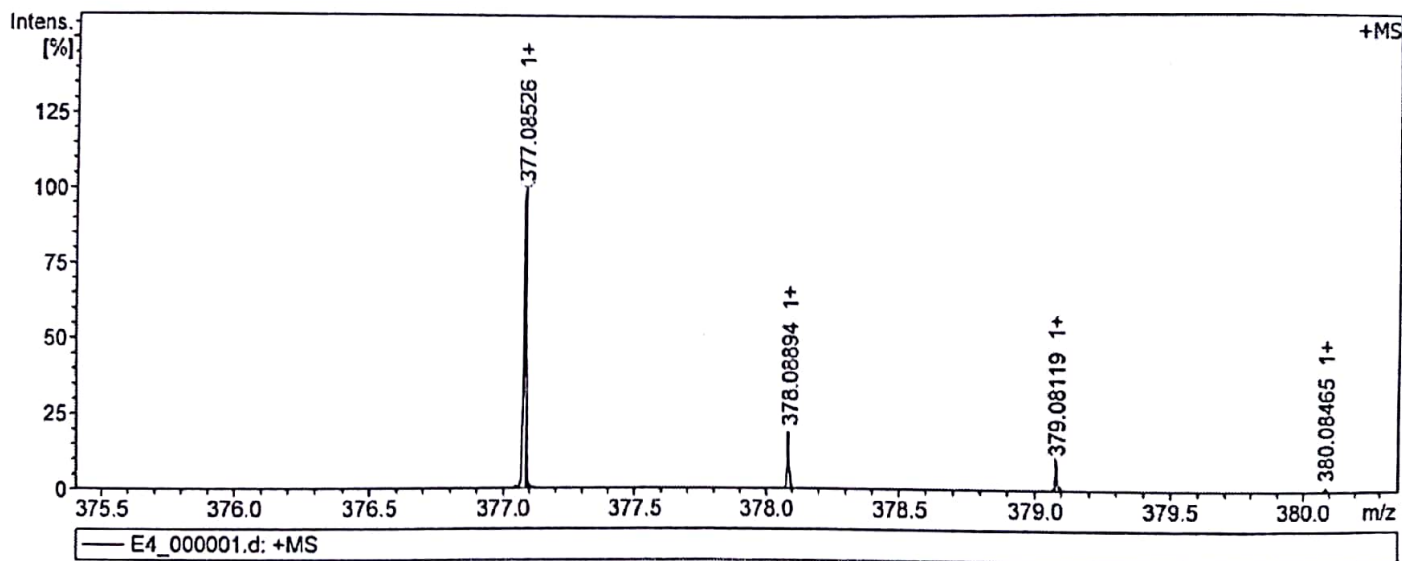
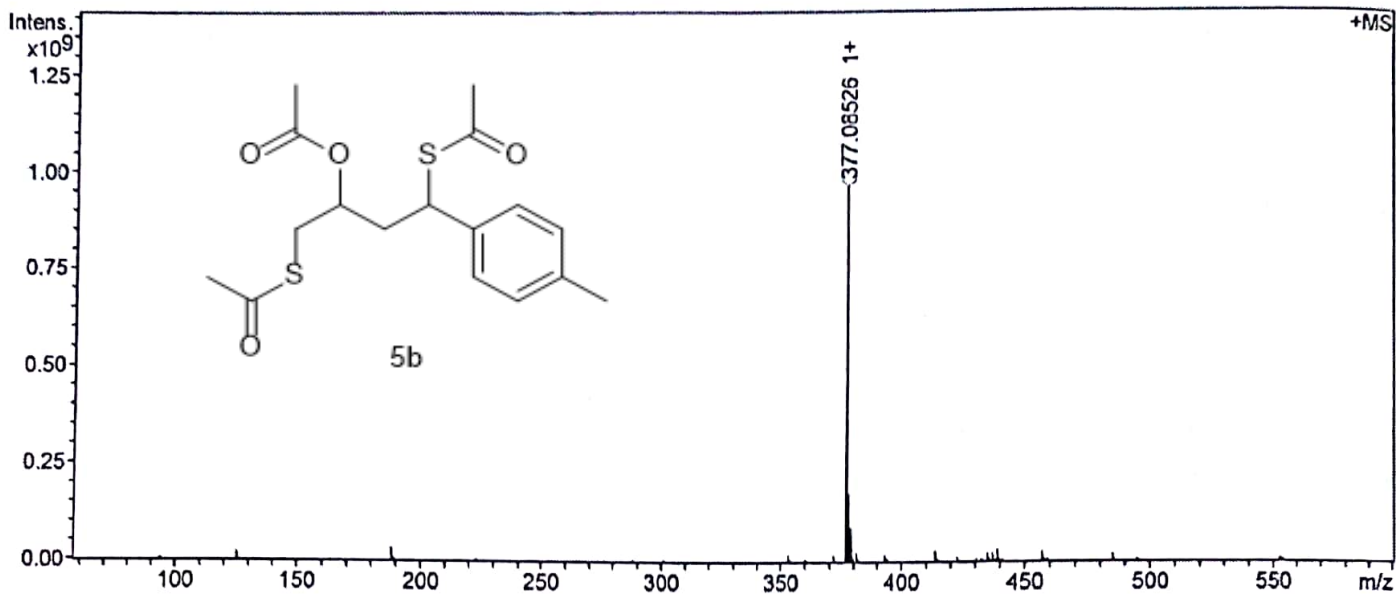
Instrument solariX

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	6	Calibration Date	Thu Mar 10 09:43:56
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	2046576
Broadband Low Mass	57.7 m/z	Source Accumulation	0.001 sec	Data Processing Size	2097152
Broadband High Mass	800.0 m/z	Ion Accumulation Time	0.200 sec	Apodization	Sine-Bell Multiplication



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
363.069199	1	C ₁₆ H ₂₀ NaO ₄ S ₂	100.00	363.069522	0.9	1.2	13.5	6.5	even	ok



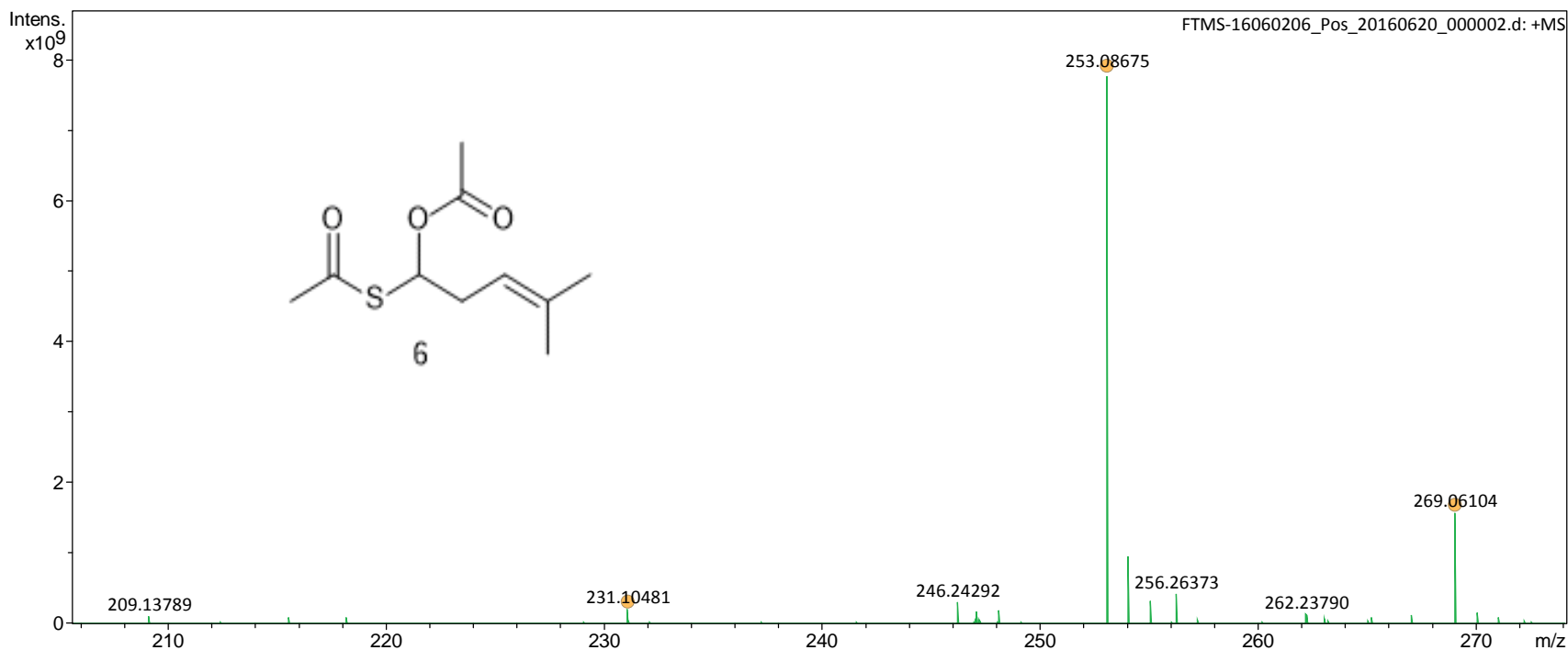
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377.085262	1	C ₁₇ H ₂₂ NaO ₄ S ₂	100.00	377.085172	-0.2	-0.0	13.7	6.5	even	ok

Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

Analysis Name FTMS-16060206_Pos_20160620_000002.d
Sample F3-2
Comment

Acquisition Date 6/20/2016 8:53:32 AM
Instrument Bruker Solarix XR FTMS
Operator Peking University



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
231.104814	1	C11H19O3S	100.00	231.104942	0.6	0.3	19.8	2.5	even		ok
253.086752	1	C11H18NaO3S	100.00	253.086886	0.5	0.2	2.7	2.5	even		ok
269.061043	1	C11H18KO3S	100.00	269.060824	-0.8	-1.1	15.0	2.5	even		ok

ESI(P),B4-1,20160318

Analysis Info

Analysis Name D:\Data\ESI\2016\2016-03\0318\B4-1_000002.d

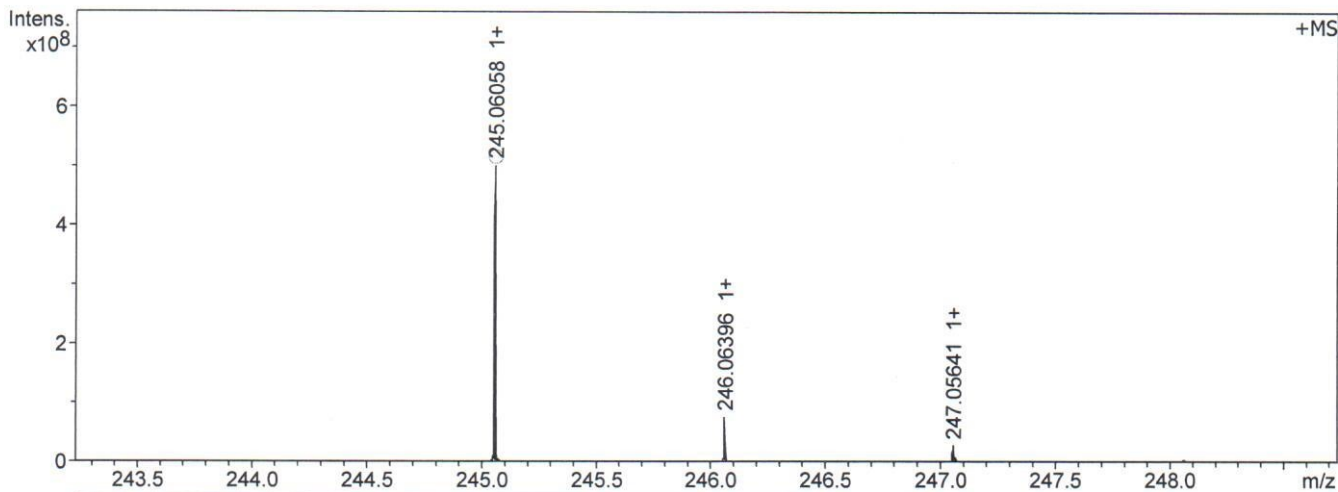
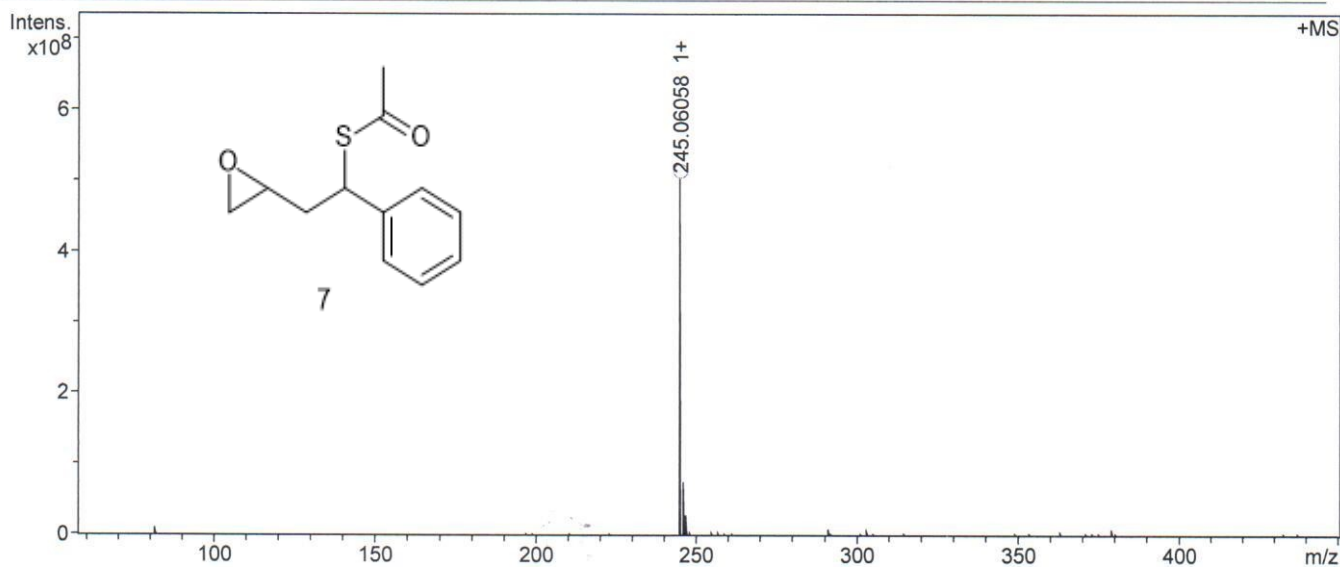
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Sample Name B4-1

Instrument solariX

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	8	Calibration Date	Thu Mar 10 09:43:56
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	2046576
Broadband Low Mass	57.7 m/z	Source Accumulation	0.001 sec	Data Processing Size	2097152
Broadband High Mass	450.0 m/z	Ion Accumulation Time	0.100 sec	Apodization	Sine-Bell Multiplication



B4-1_000002.d: +MS

Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
245.060583	1	C12H14NaO2S	100.00	245.060671	0.4	0.3	27.6	5.5	even	ok

ESI(P),B4,20170426

Analysis Info

Analysis Name D:\Data\ESI\2017\2017-04\0426\B4_000001.d

Sample Name B4

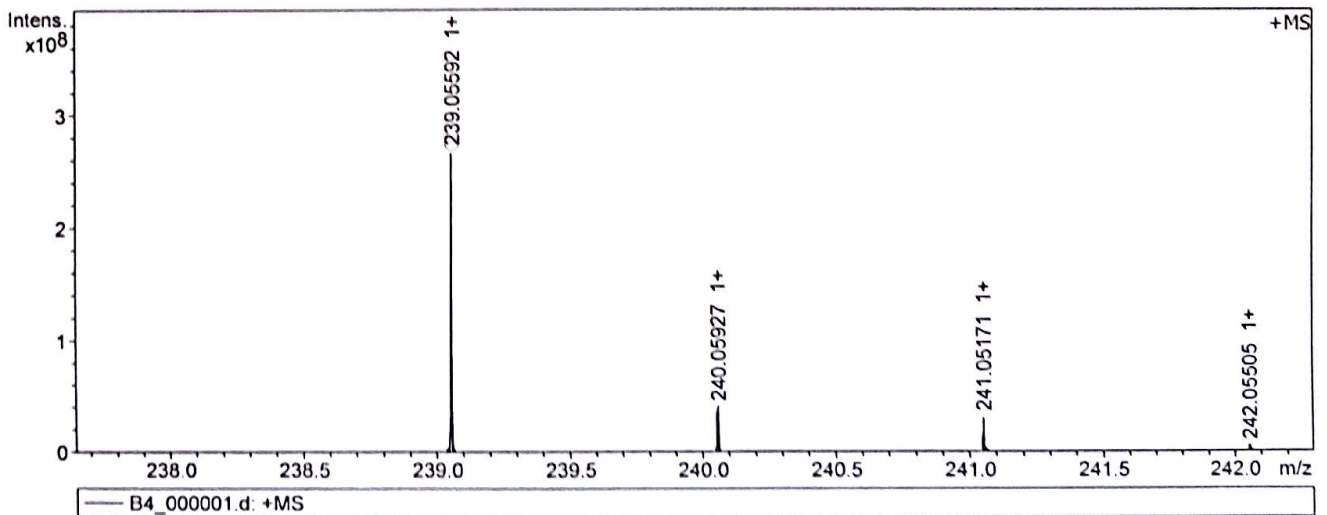
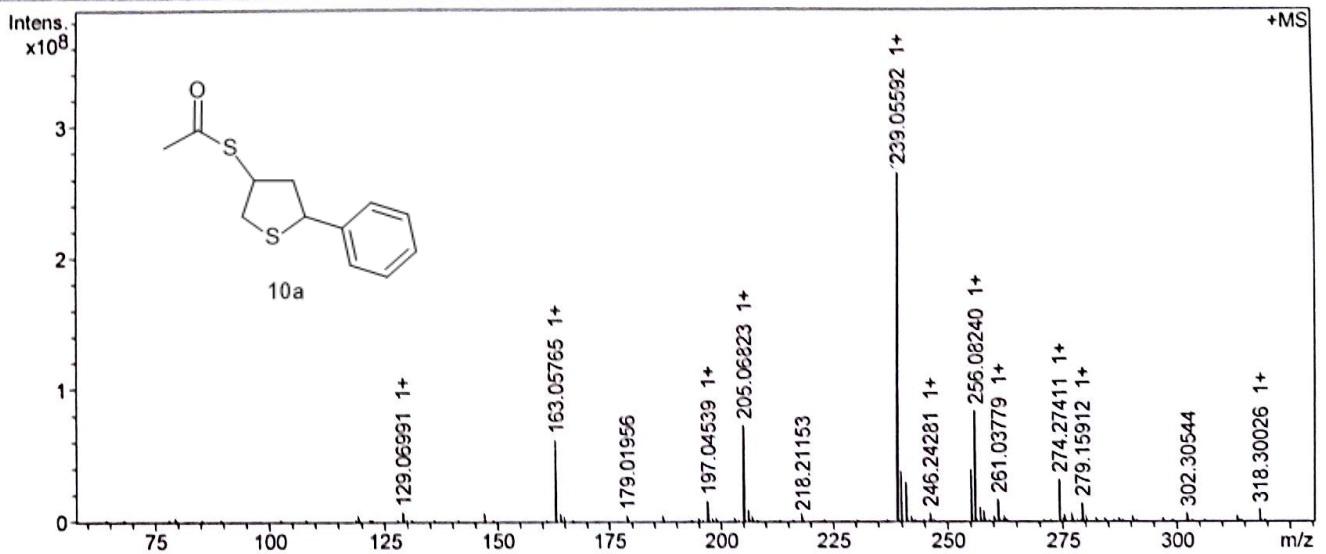
Acquisition Date 4/26/2017 10:39:30 AM

Operator
Instrument solariX

Acquisition Parameter

Polarity Positive
Broadband Low Mass 57.7 m/z
Broadband High Mass 330.0 m/z

Calibration Date Thu Apr 13 09:19:13 2017
Acquired Scans 10



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
239.055920	1	C12H15OS2	100.00	239.055884	-0.2	0.1	7.3	5.5	even	ok

ESI(P),E4,20170526

Analysis Info

Analysis Name D:\Data\ESI\2017\2017-05\0526\E4_000001.d

Sample Name E4

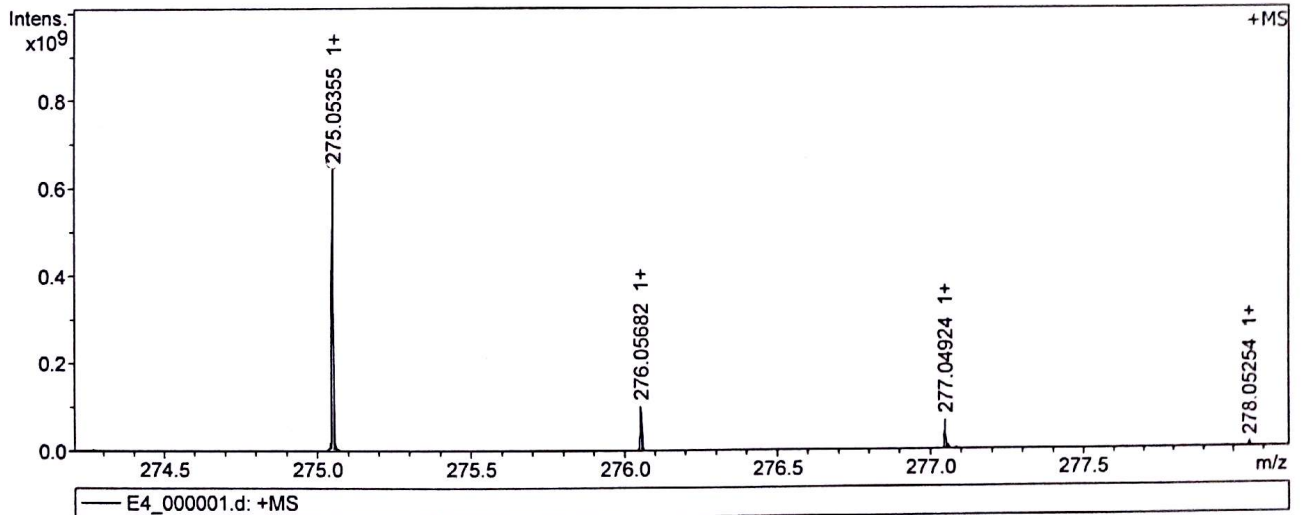
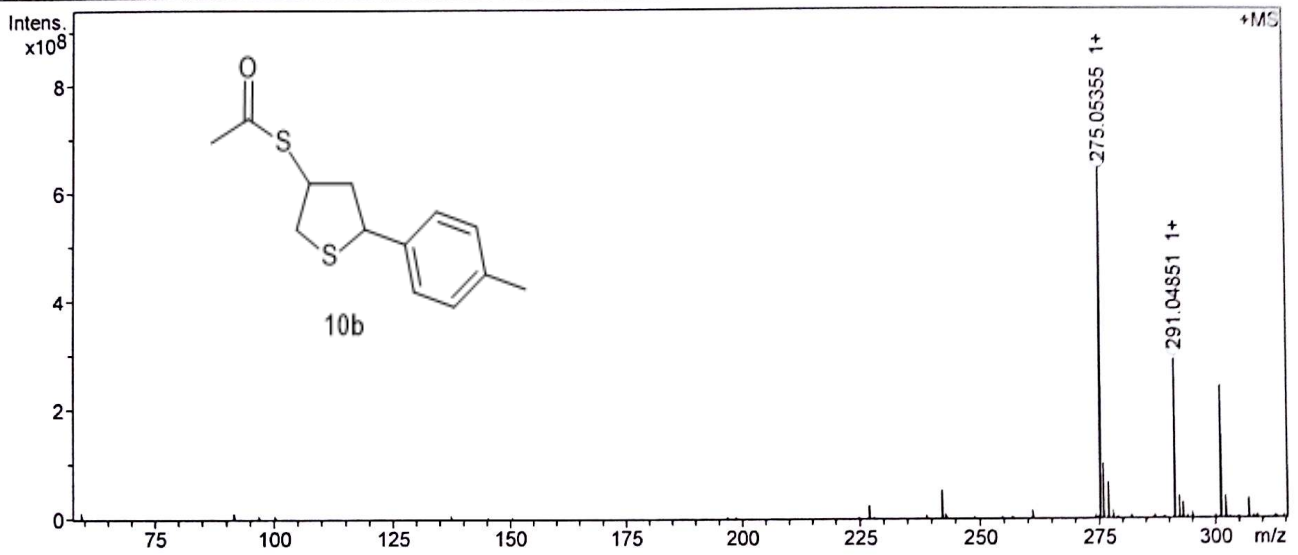
Acquisition Date 5/26/2017 9:56:59 AM

Operator
Instrument solariX

Acquisition Parameter

Polarity Positive
Broadband Low Mass 57.7 m/z
Broadband High Mass 315.0 m/z

Calibration Date Mon May 8 09:15:29
2017
Acquired Scans 10



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
275.053554	1	C ₁₃ H ₁₆ NaOS ₂	100.00	275.053478	0.3	0.1	1.8	5.5	even	ok
291.048510	1	C ₁₃ H ₁₆ NaO ₂ S ₂	100.00	291.048392	-0.4	-0.1	8.0	5.5	even	ok

ESI(P),B2-S,20171025

Analysis Info

Analysis Name D:\Data\ESI\2017\2017-10\1025\B2-S_000001.d

Sample Name B2-S

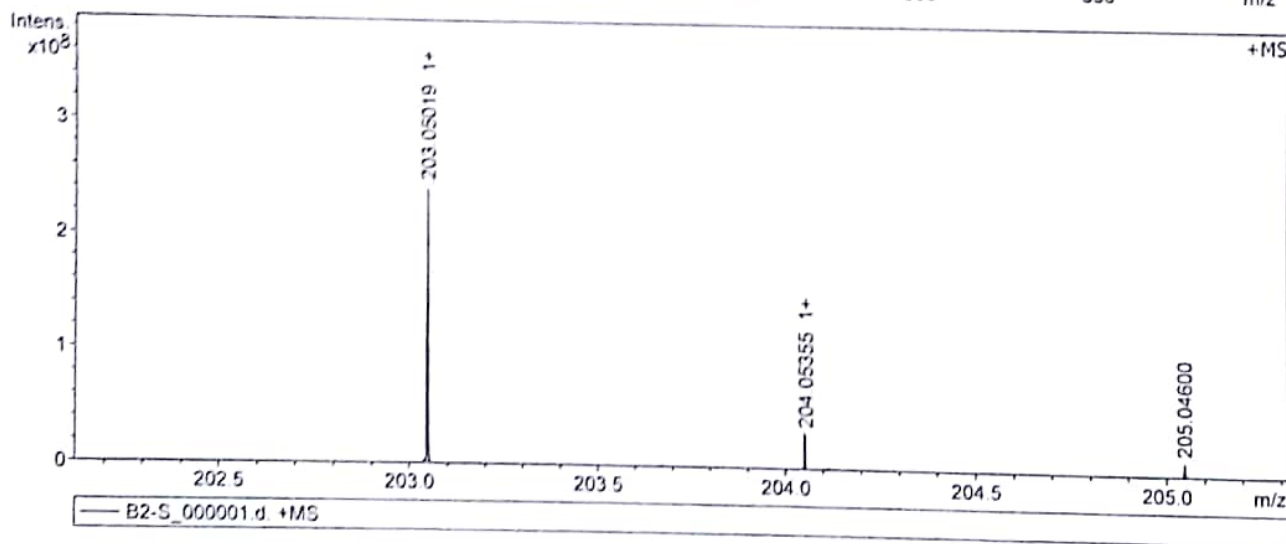
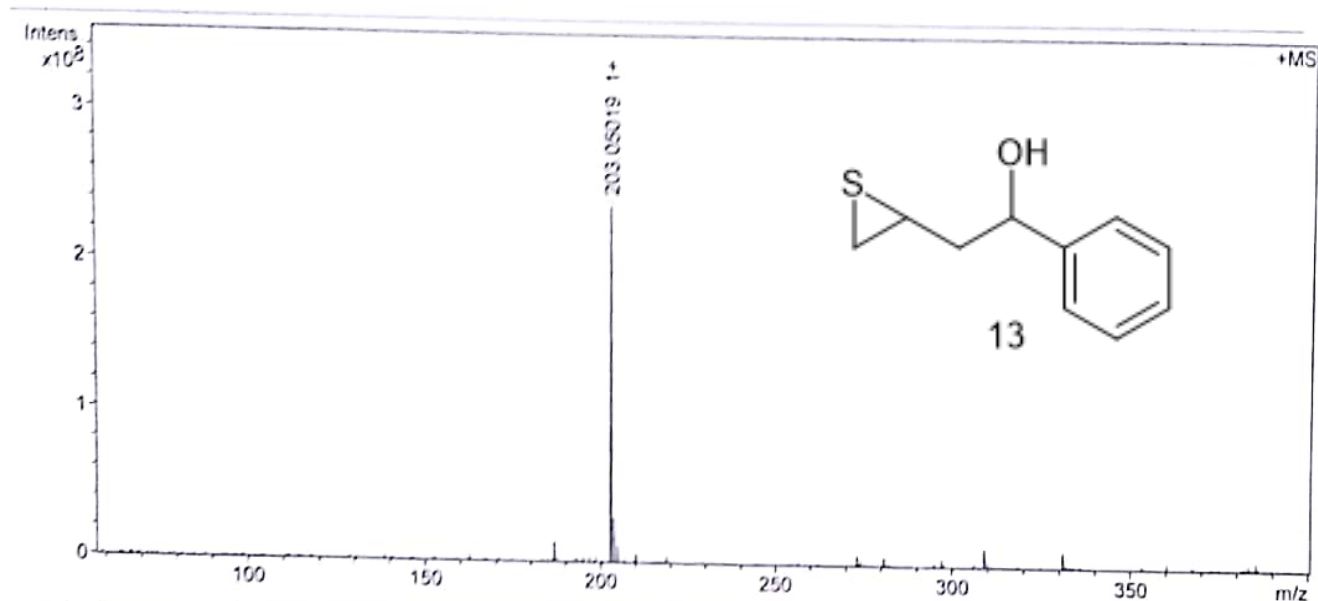
Acquisition Date 10/25/2017 10:56:48 AM

Operator
Instrument solariX

Acquisition Parameter

Polarity Positive
Broadband Low Mass 57.7 m/z
Broadband High Mass 400.0 m/z

Calibration Date Fri Sep 22 03:00:05 2017
Acquired Scans 10



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
203.050192	1	C ₁₀ H ₁₂ NaOS	100.00	203.050107	0.4	-0.2	5.8	4.5	even	ok

ESI(P),B3-S,20171025

Analysis Info

Analysis Name D:\Data\ESI\2017\2017-10\1025\B3-S_000002.d

Sample Name B3-S

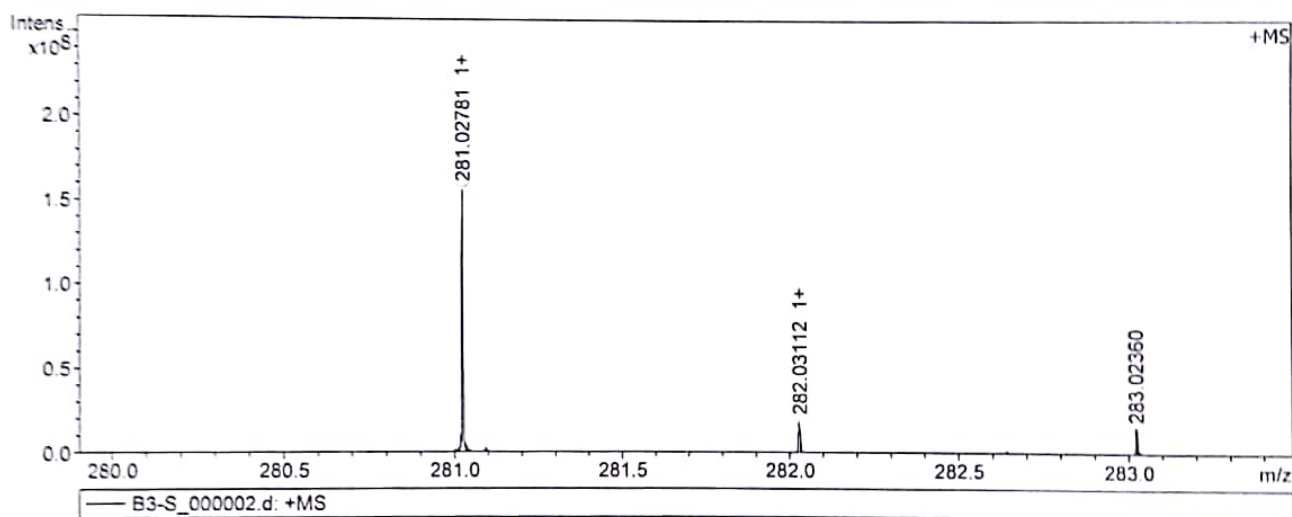
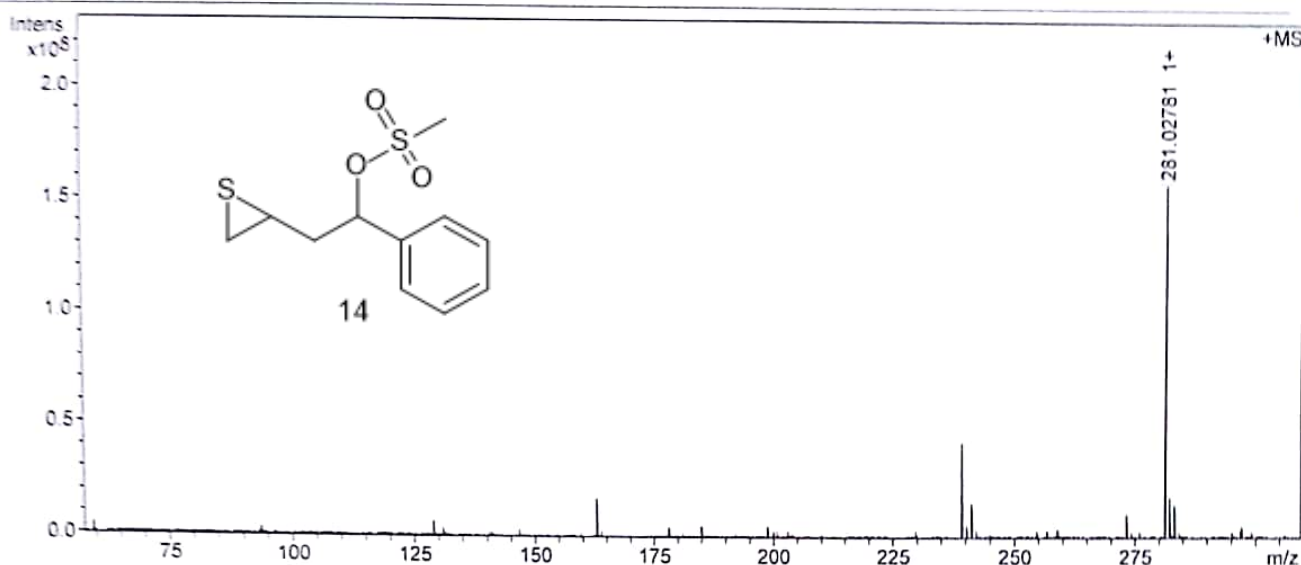
Acquisition Date 10/25/2017 10:50:53 AM

Operator
Instrument solariX

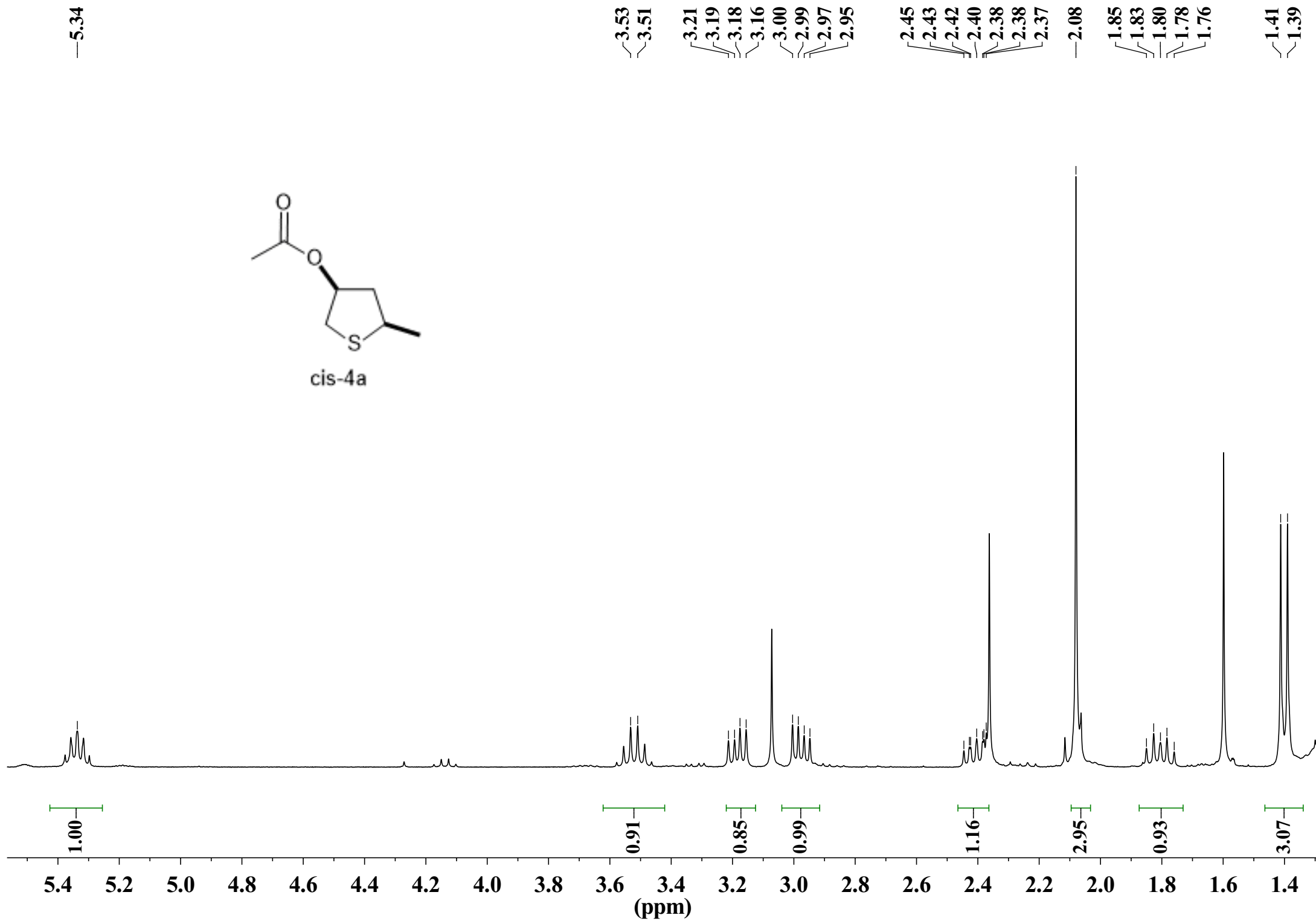
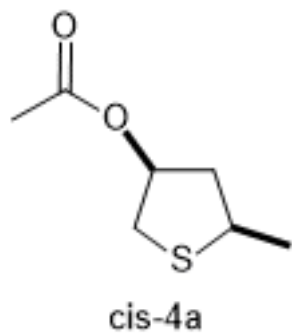
Acquisition Parameter

Polarity Positive
Broadband Low Mass 57.7 m/z
Broadband High Mass 309.0 m/z

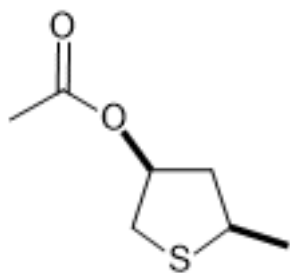
Calibration Date Fri Sep 22 03:00:05 2017
Acquired Scans 10



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
281.027809	1	C11H14NaO3S2	100.00	281.027657	0.5	-0.3	10.6	4.5	even	ok



—170.50

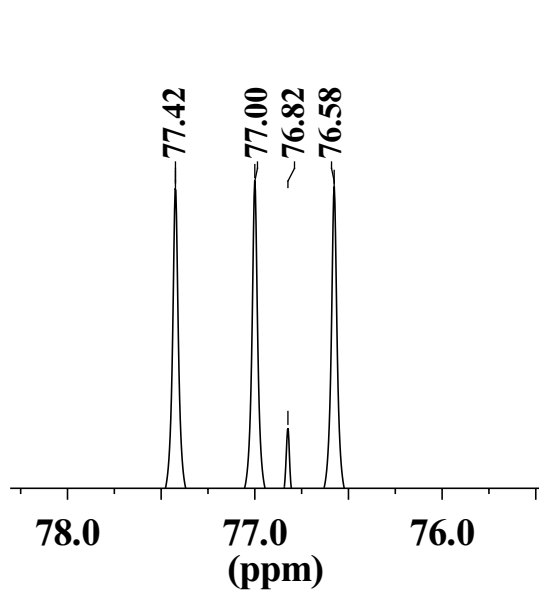


cis-4a

77.42
77.00
76.82
76.58

~43.00
~39.52
~36.41

~23.14
~21.12



180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
(ppm)

5.53
5.53
5.52
5.51
5.51
5.50
5.49

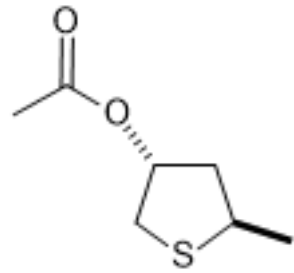
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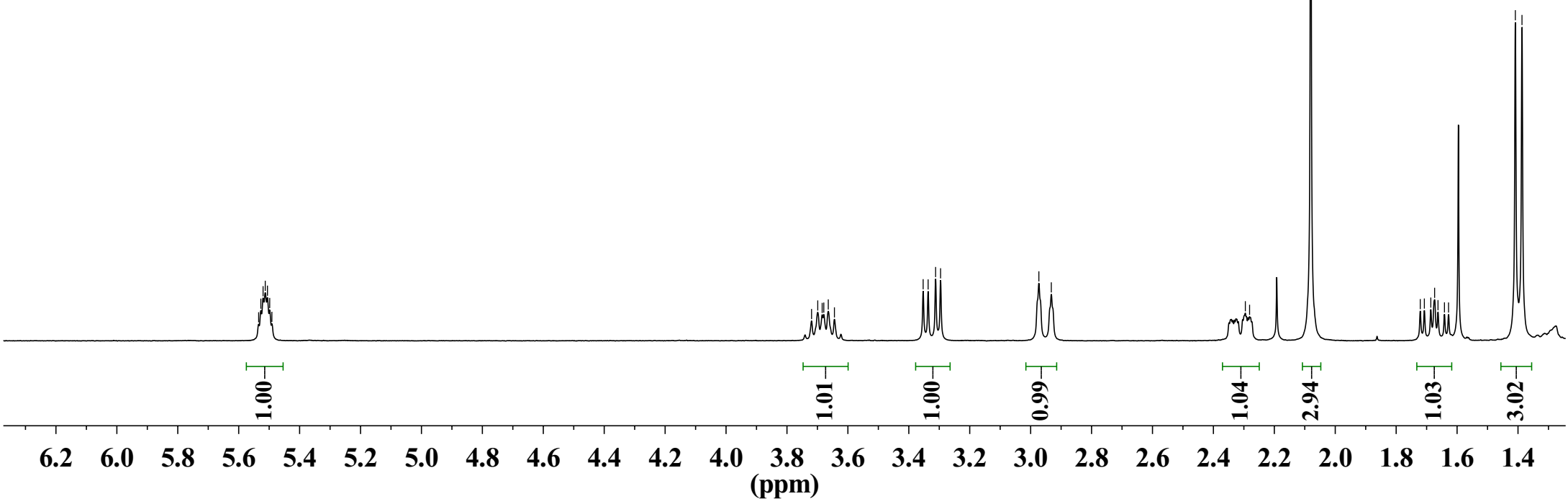
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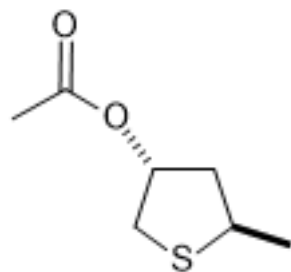
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1.41
1.39

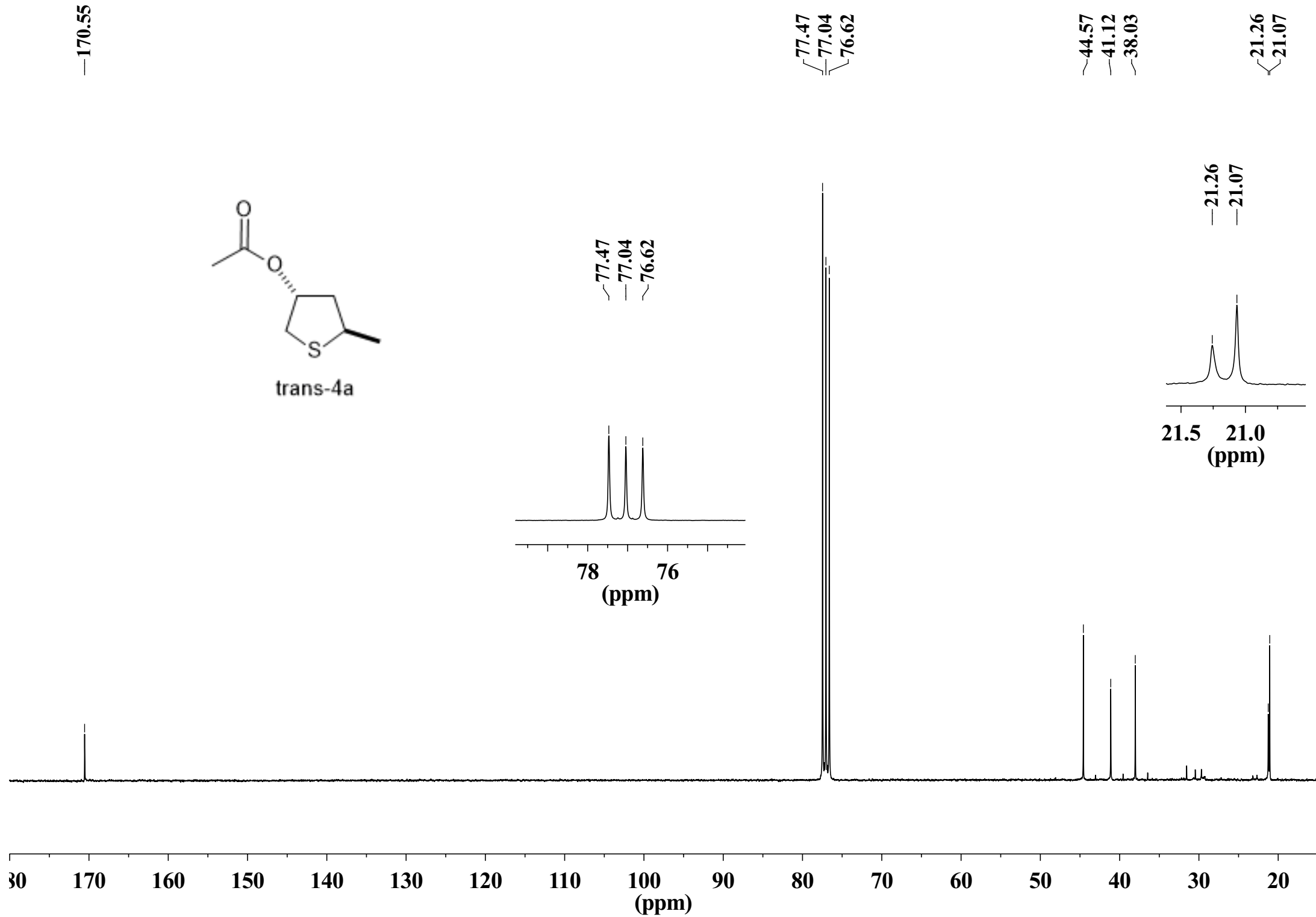


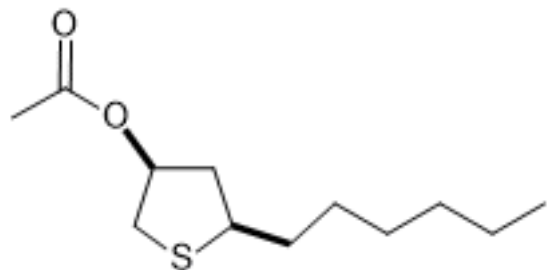
trans-4a



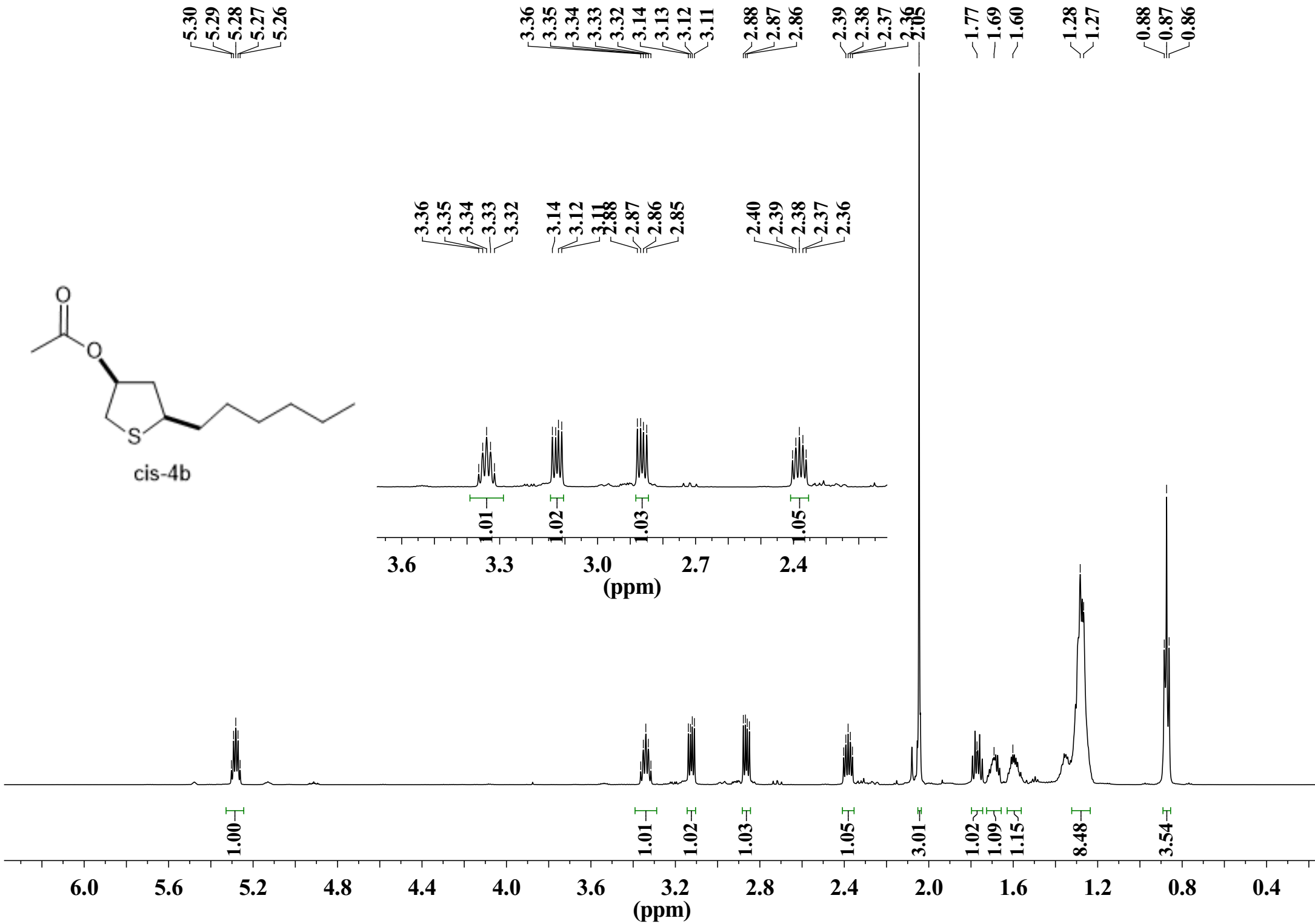


trans-4a

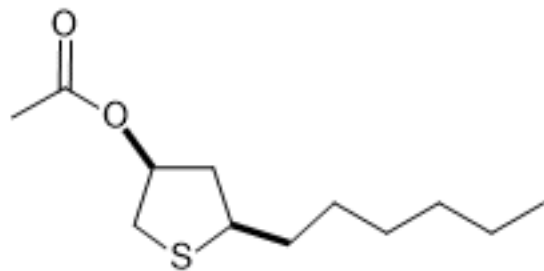




cis-4b



—170.44



cis-4b

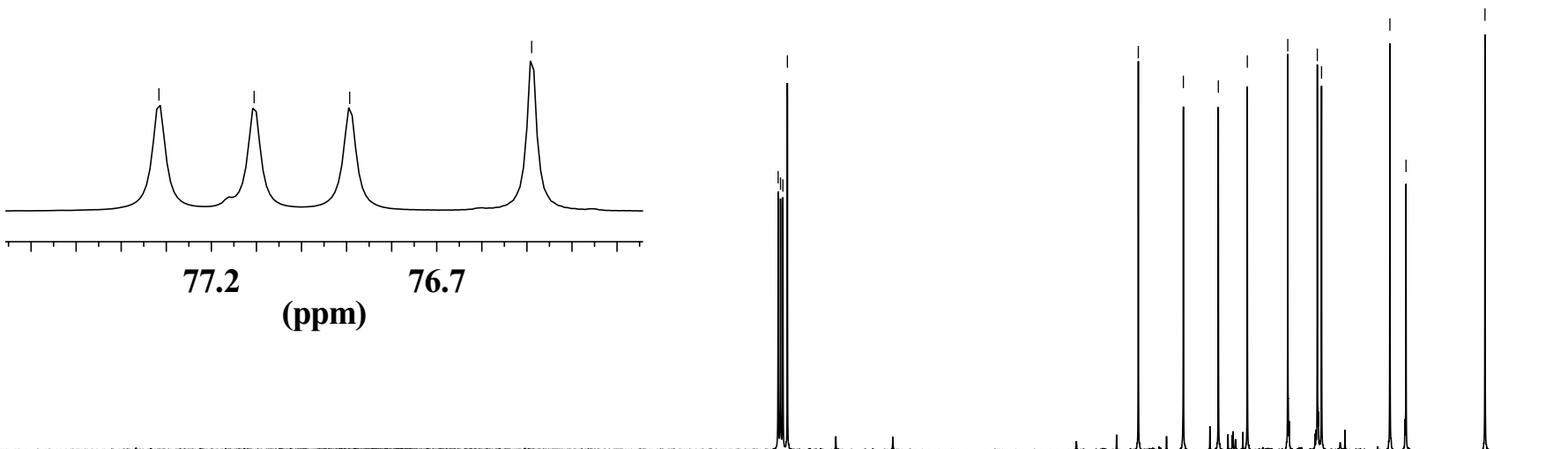
77.32
77.11
76.89
76.49

45.07
41.04
37.91
35.31
31.69
29.04
28.67

22.55
21.10

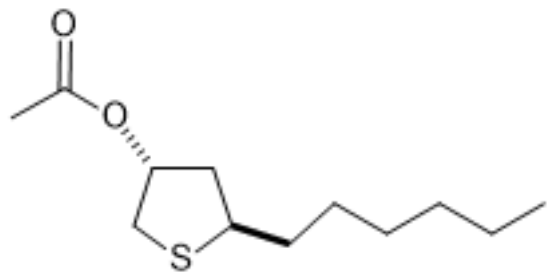
—14.03

77.32
77.11
76.89
76.49

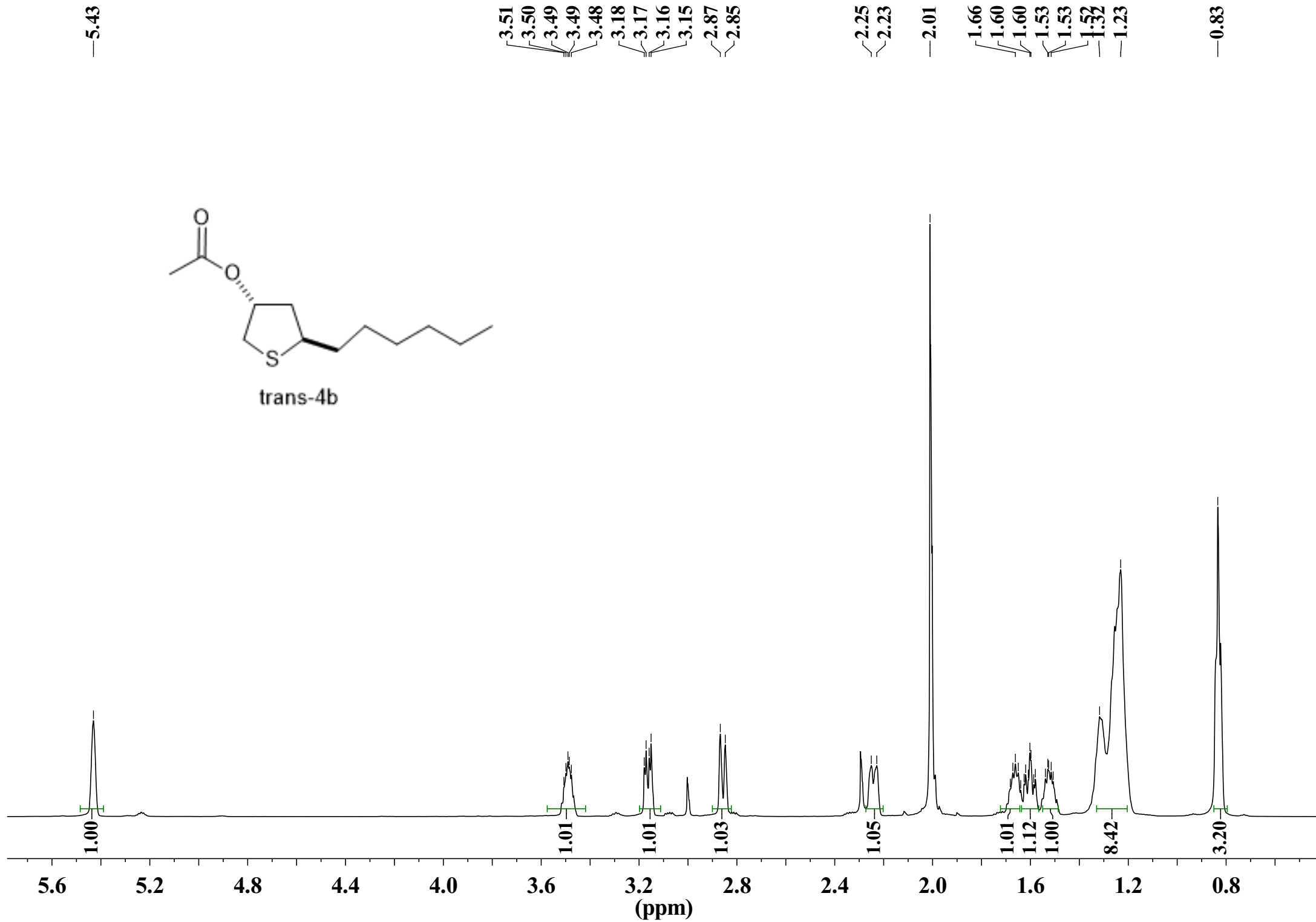


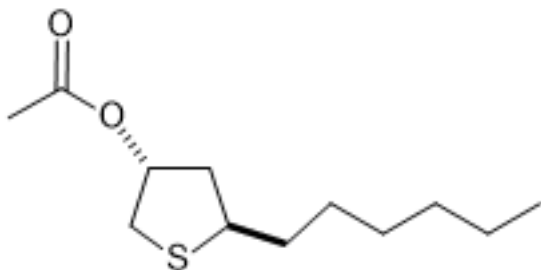
77.2
76.7
(ppm)

170 160 150 140 130 120 110 100 90 (ppm) 80 70 60 50 40 30 20 10

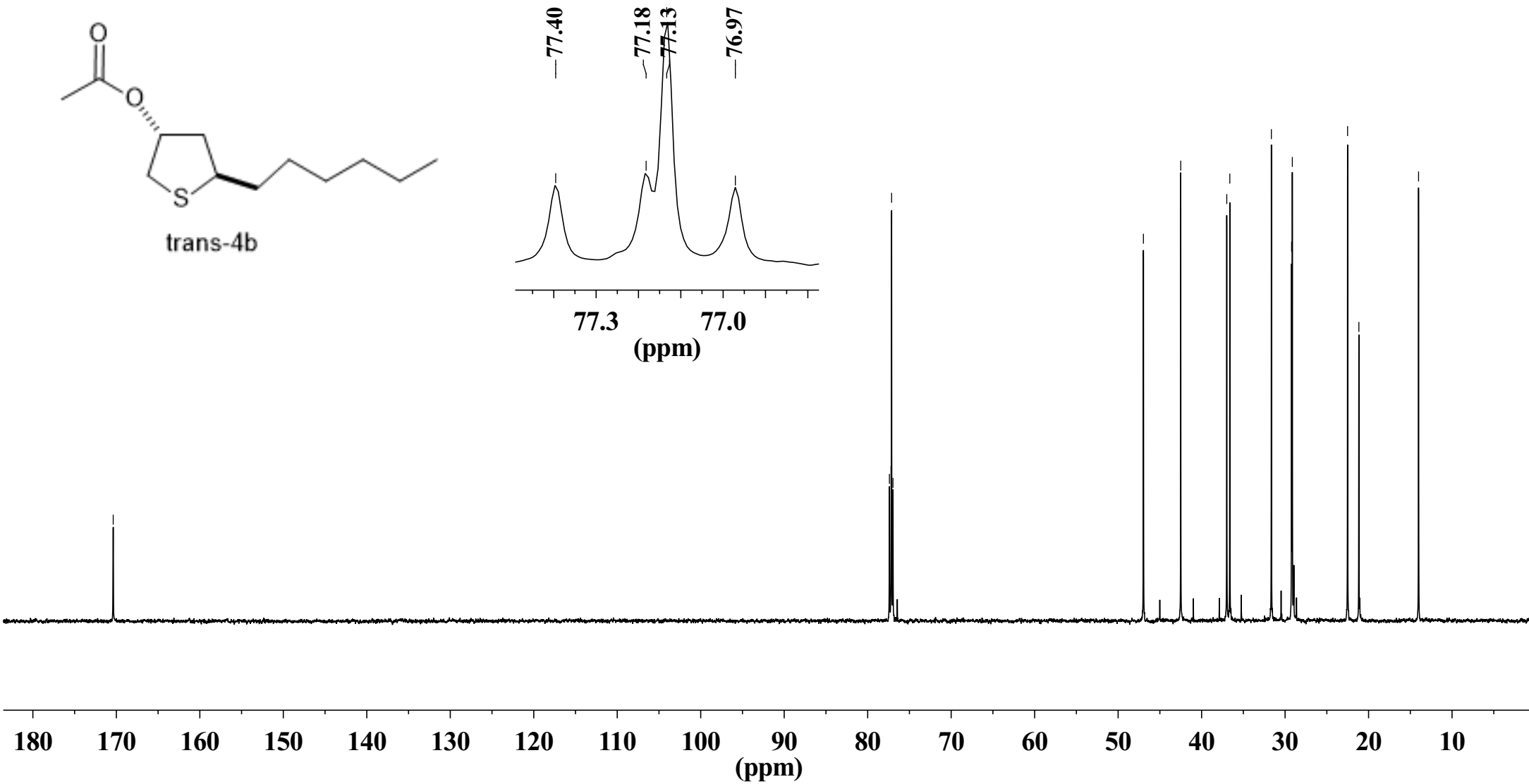


trans-4b





trans-4b



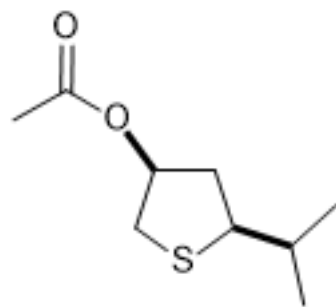
5.26
5.24
5.21
5.19
5.16

3.13
3.12
3.10
3.08
3.06

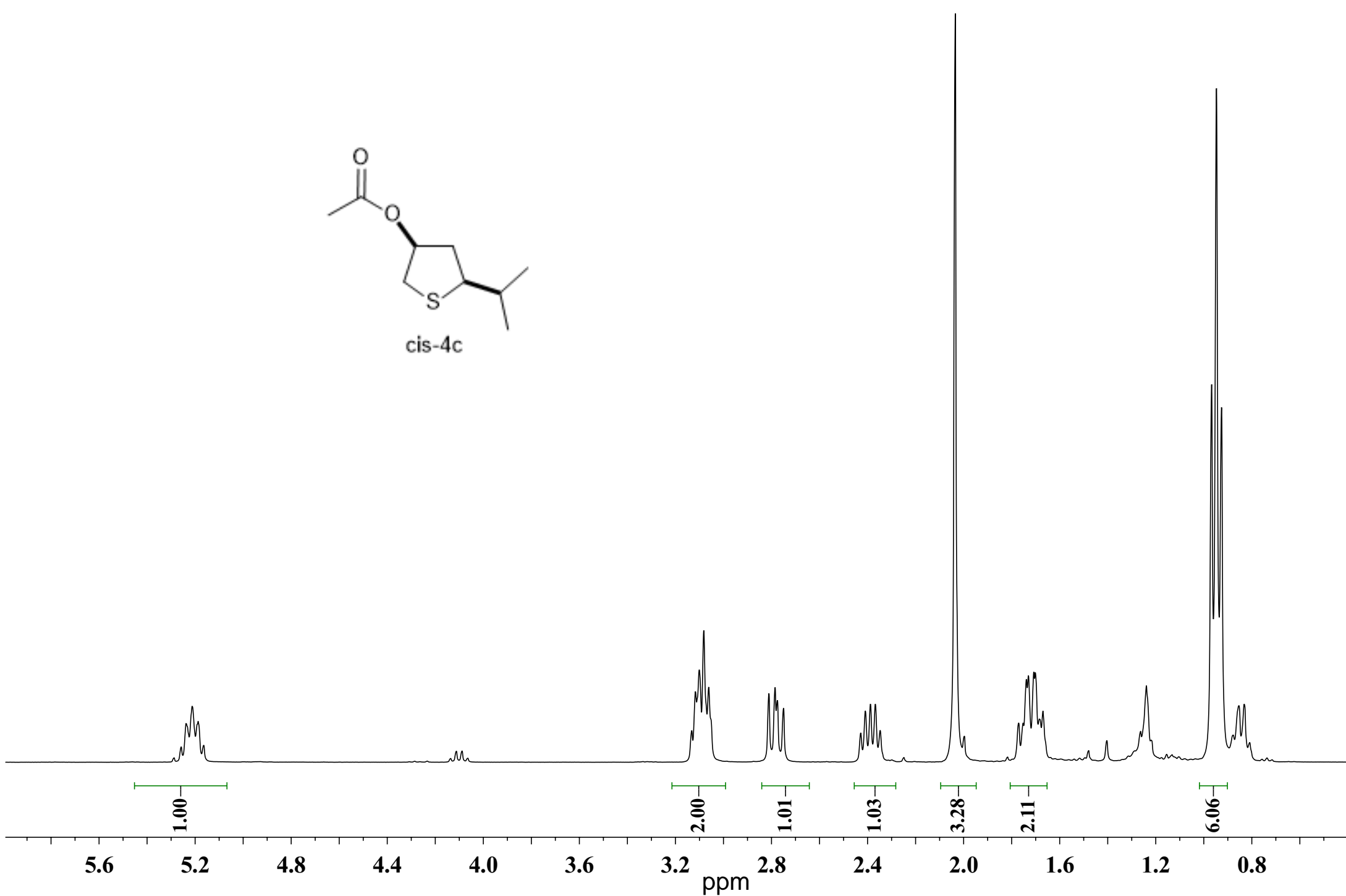
2.81
2.79
2.78
2.41
2.39
2.37
2.35

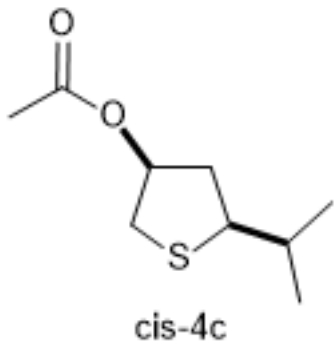
2.03
1.77
1.75
1.74
1.73
1.71
1.70
1.68
1.67

0.97
0.95
0.93

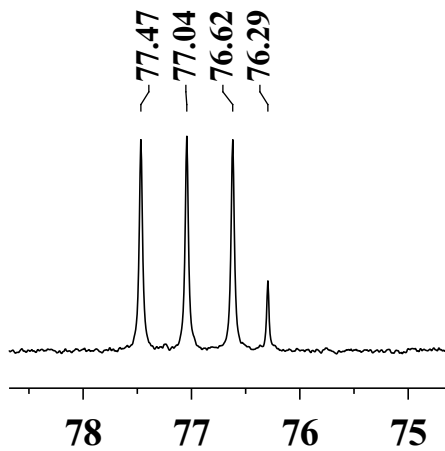


cis-4c





—170.55



77.47
77.04
76.62
76.29

—51.79

38.53

34.94

34.58

21.43

21.10

20.90

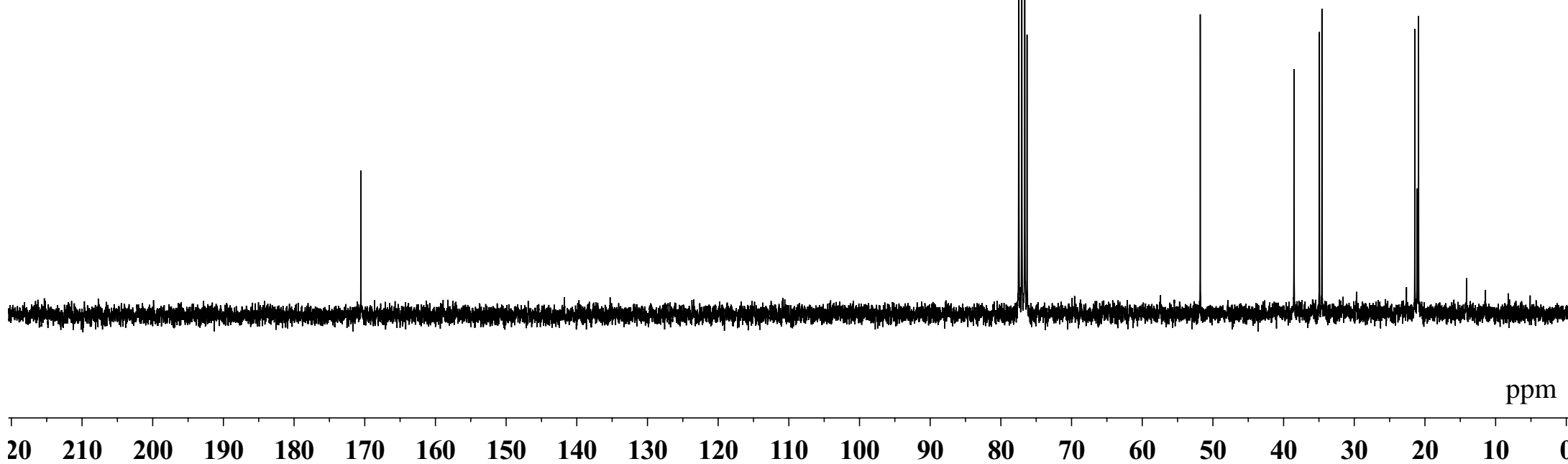
21.43

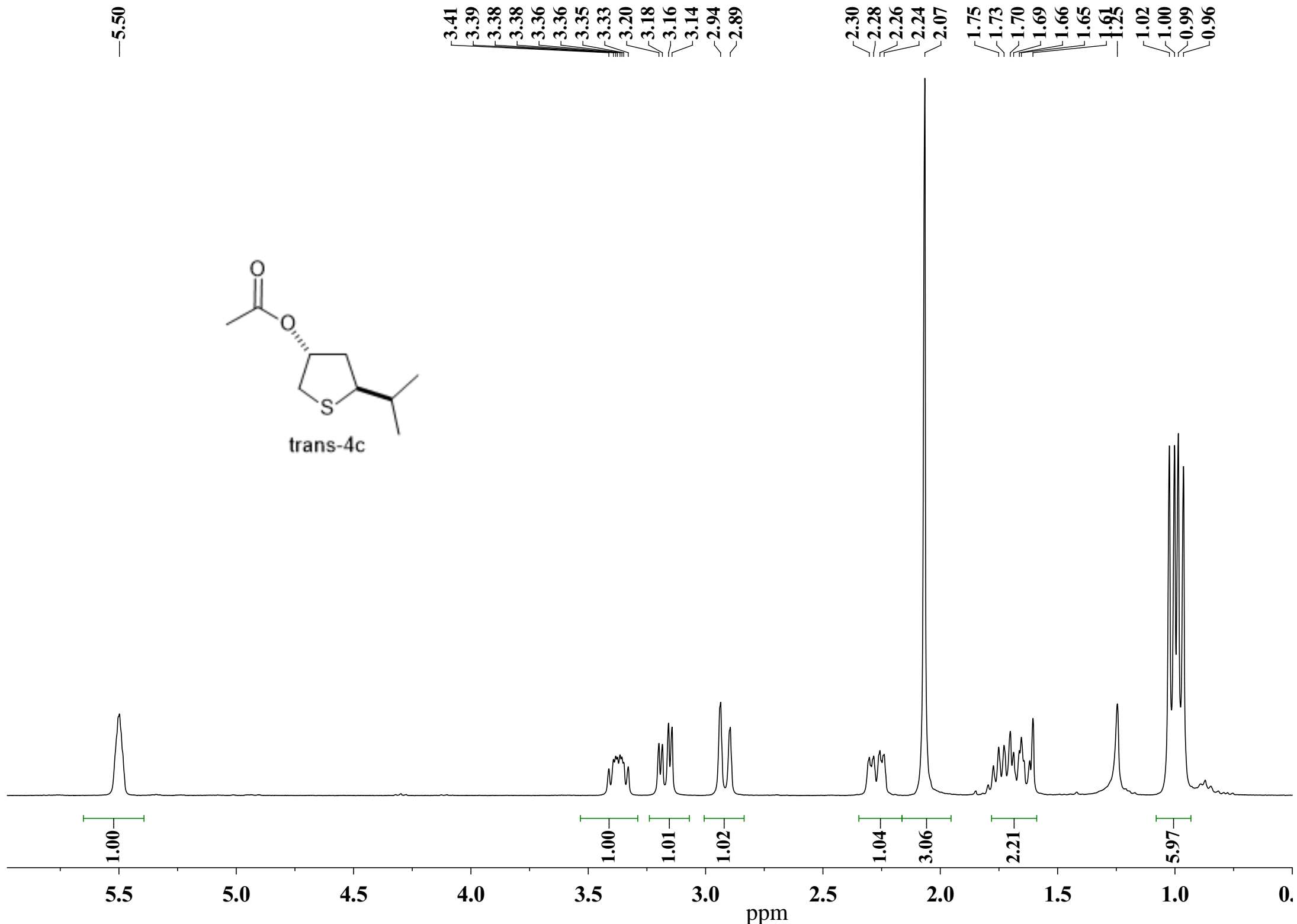
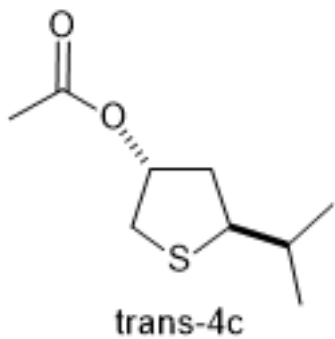
21.10

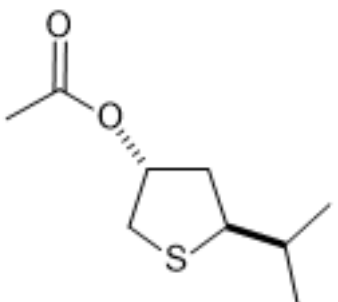
20.90

22.0

21.0







—170.60

77.60
77.41
76.98
76.56

—54.78

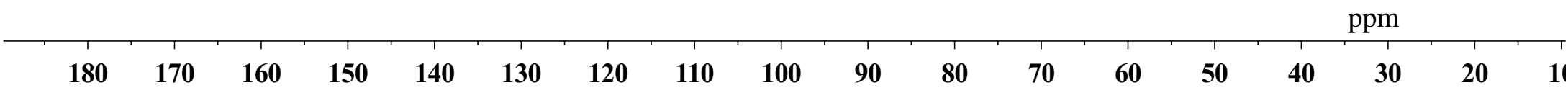
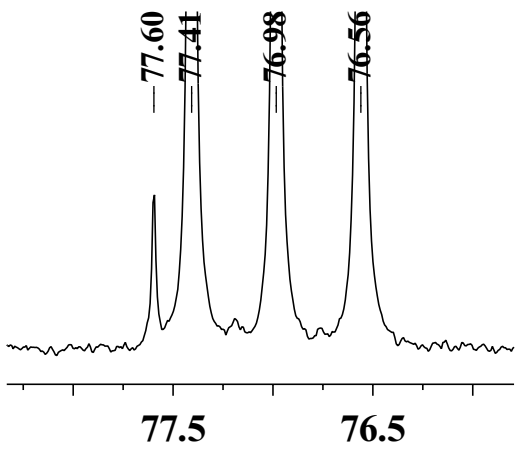
—40.33

—37.10

—34.41

—22.18

—21.29



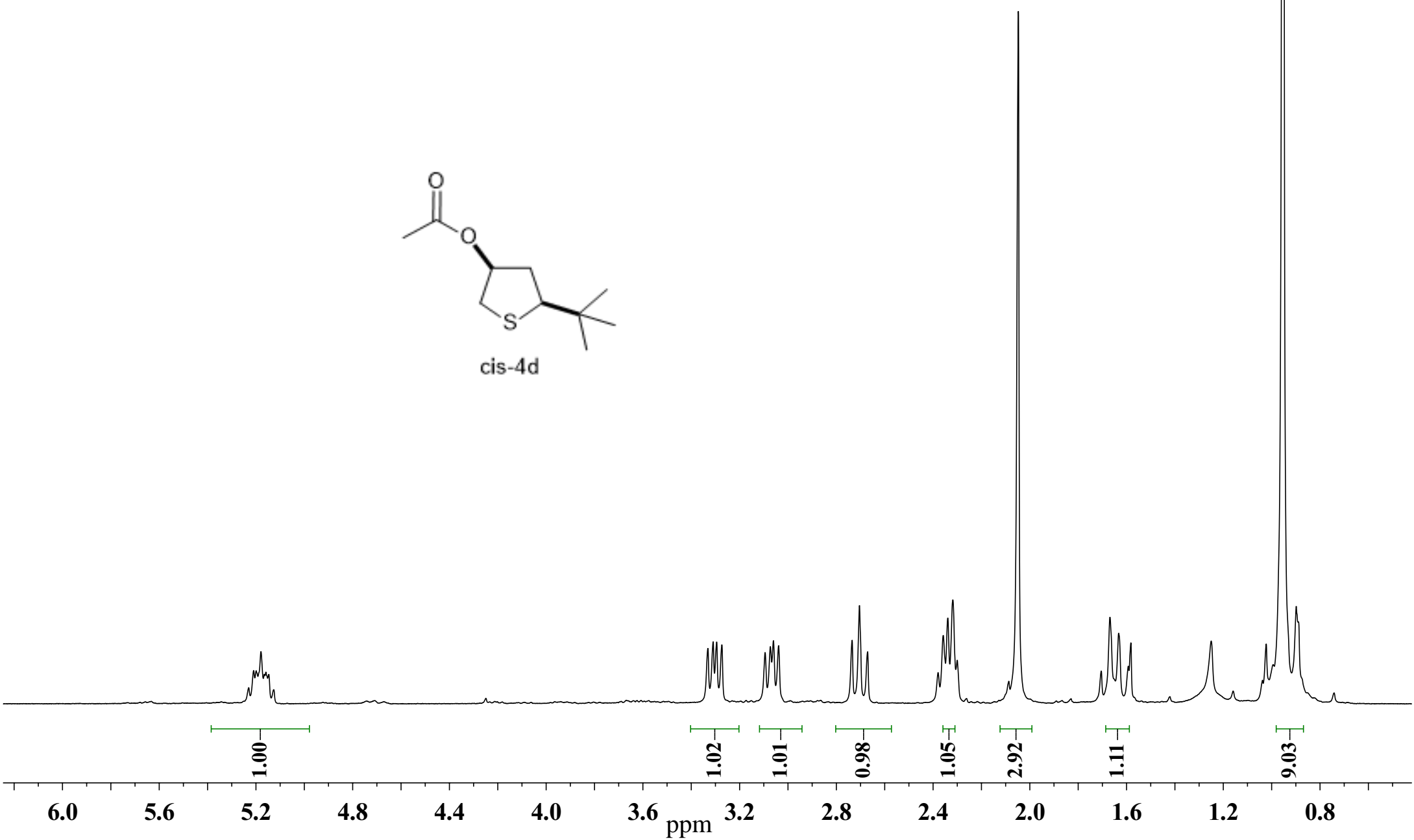
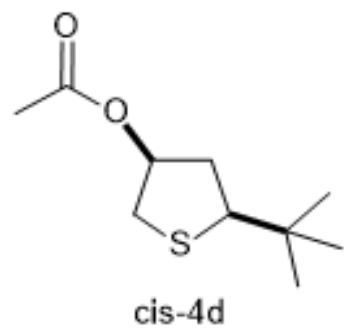
5.23
5.21
5.20
5.18
5.17
5.16
5.15
5.13

3.33
3.31
3.29
3.27
3.09
3.07
3.06
3.04
2.73
2.70
2.67

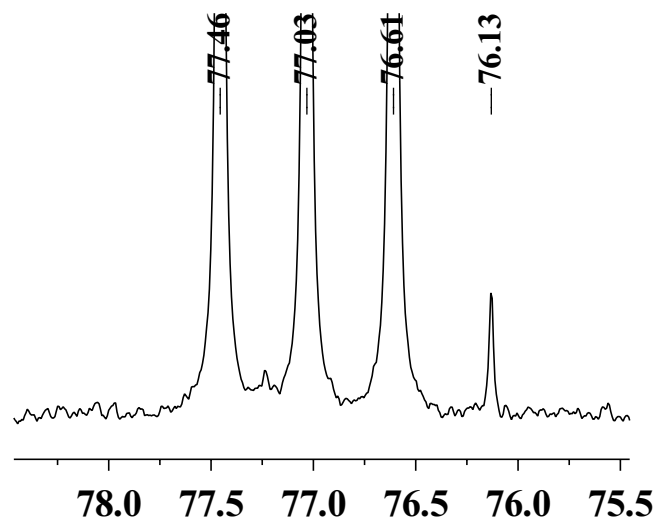
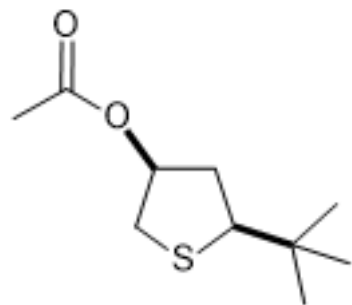
2.36
2.34
2.32
2.30
2.05

1.70
1.67
1.63
1.59
1.58

0.95



—170.61



77.46
77.03
76.61
76.13

—55.10

35.26
34.13
33.78

—27.10

—21.11

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20

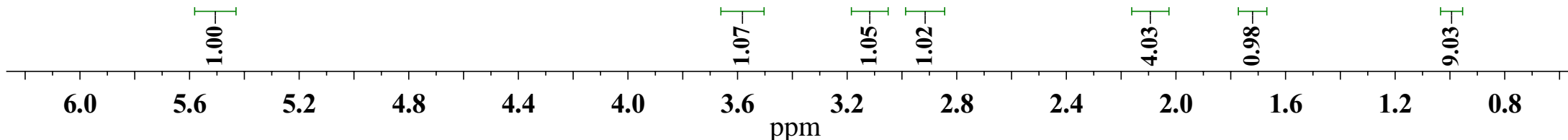
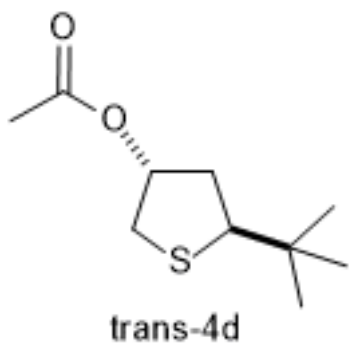
ppm

—5.49

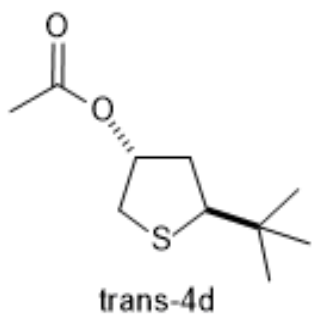
3.60
3.58
3.56
3.54
3.13
3.12
3.09
3.08
2.93
2.89

2.15
2.13
2.08
2.05
1.76
1.75
1.72
1.71
1.68
1.67

0.98



—170.70



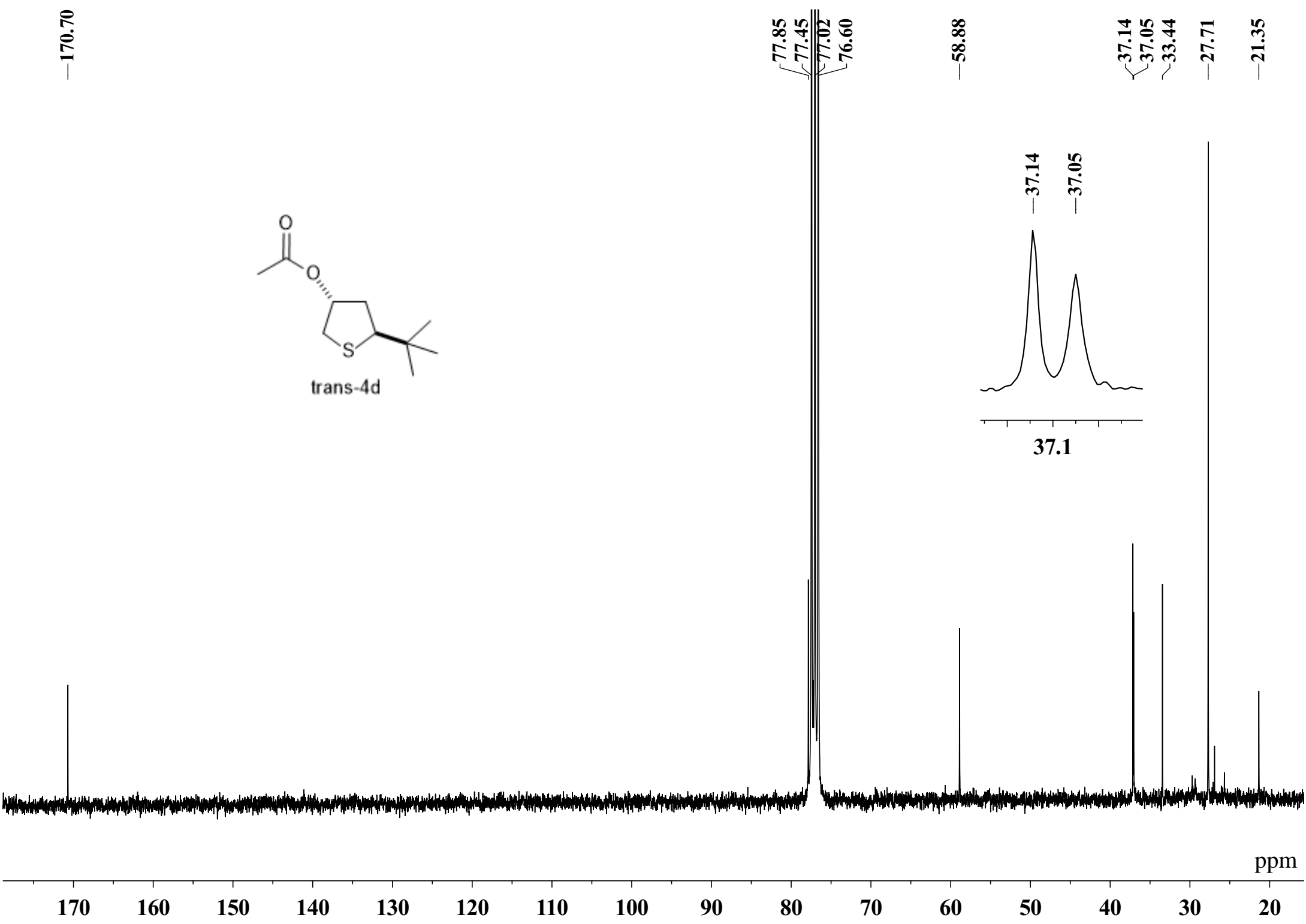
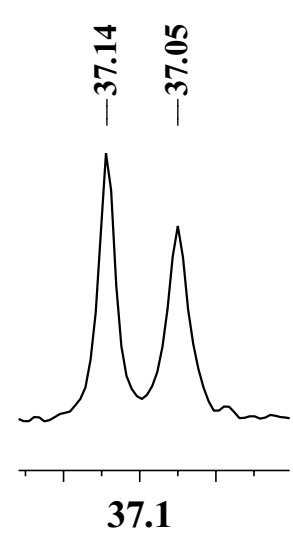
77.85
77.45
77.02
76.60

—58.88

37.14
37.05
33.44

—27.71

—21.35

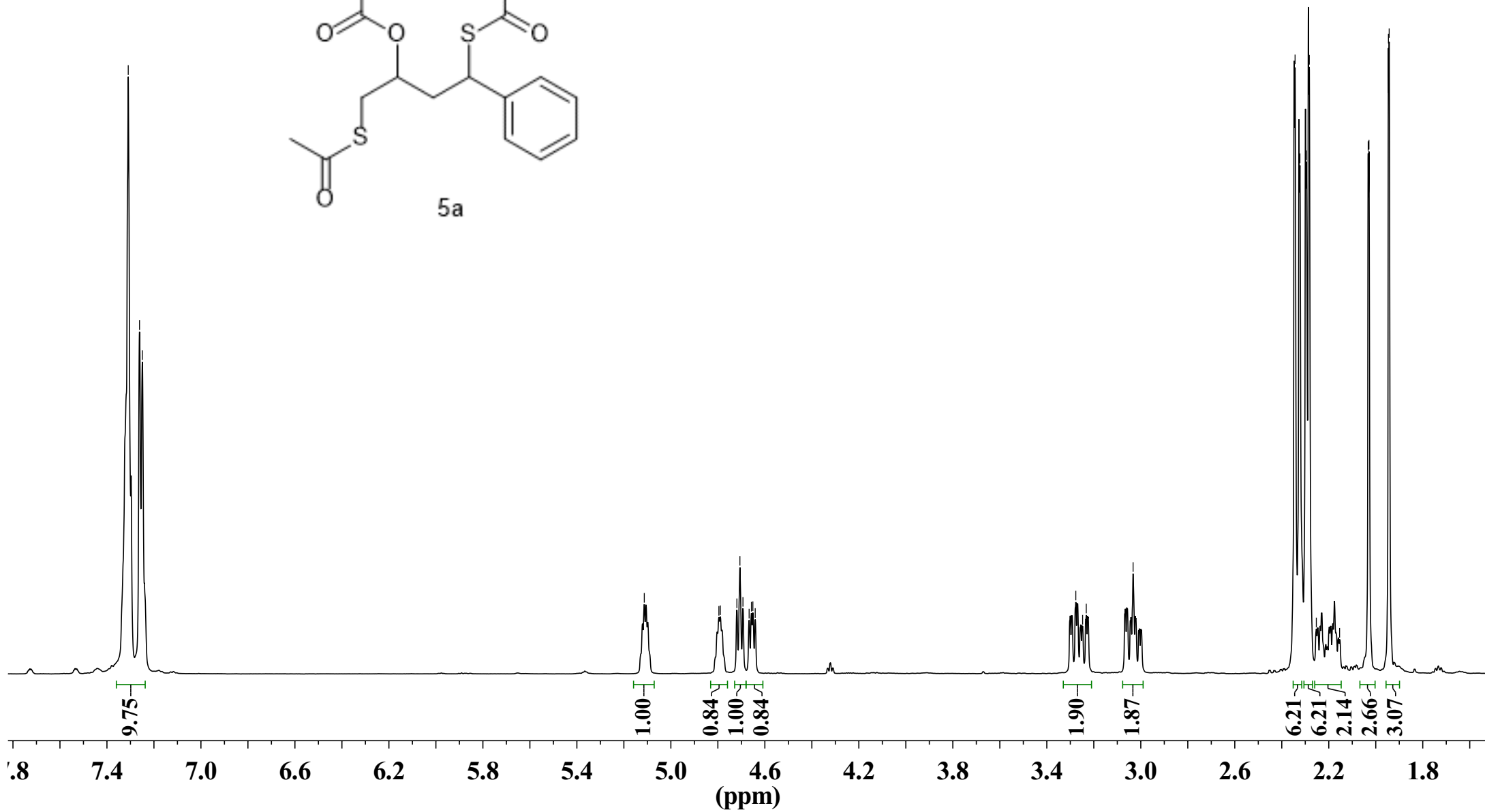
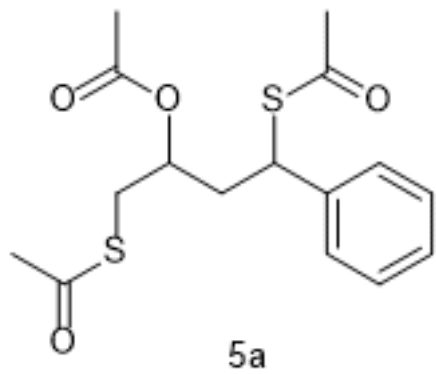


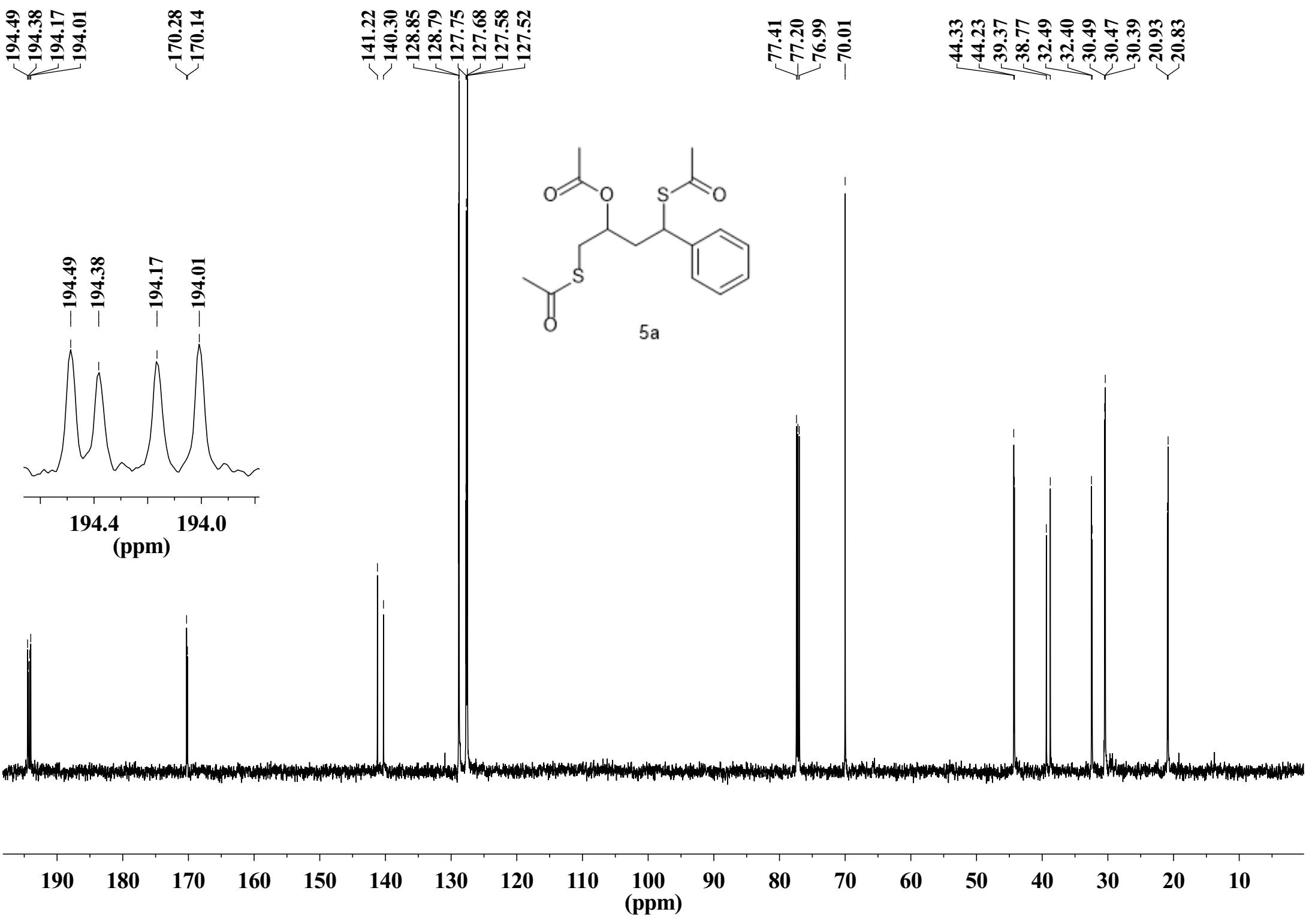
7.31
7.26
7.25

5.11
4.80
4.79
4.72
4.71
4.69
4.67
4.66
4.65
4.64

3.28
3.25
3.23
3.03

2.34
2.32
2.30
2.28
2.25
2.15
2.03
2.03
1.95
1.94



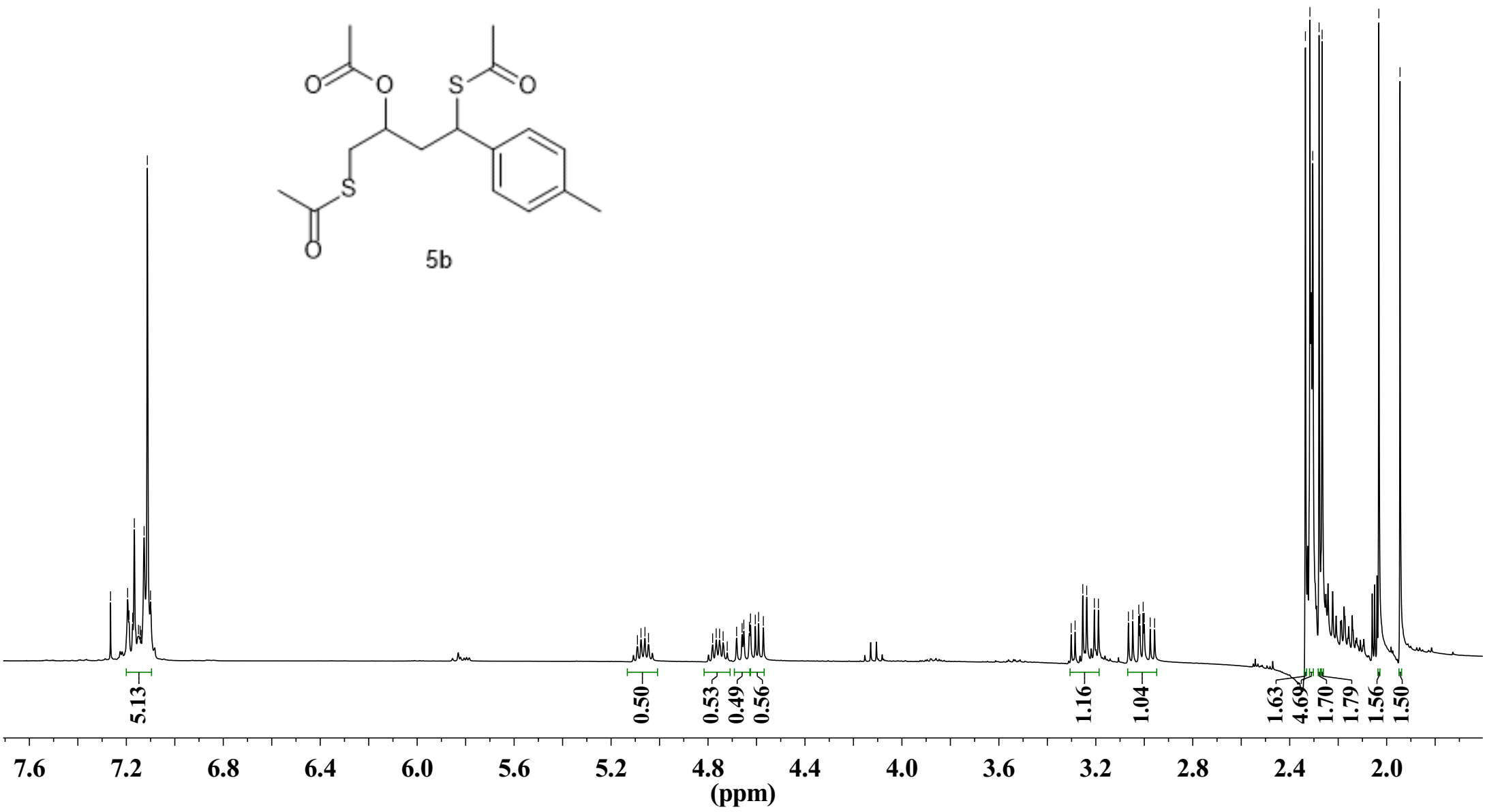
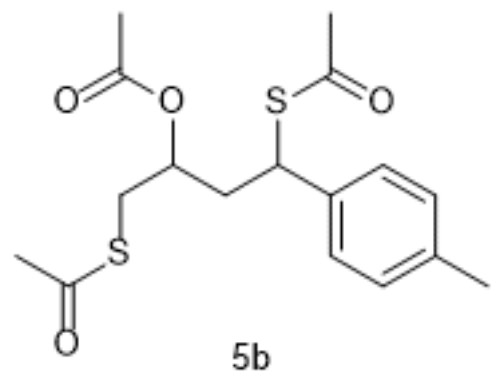


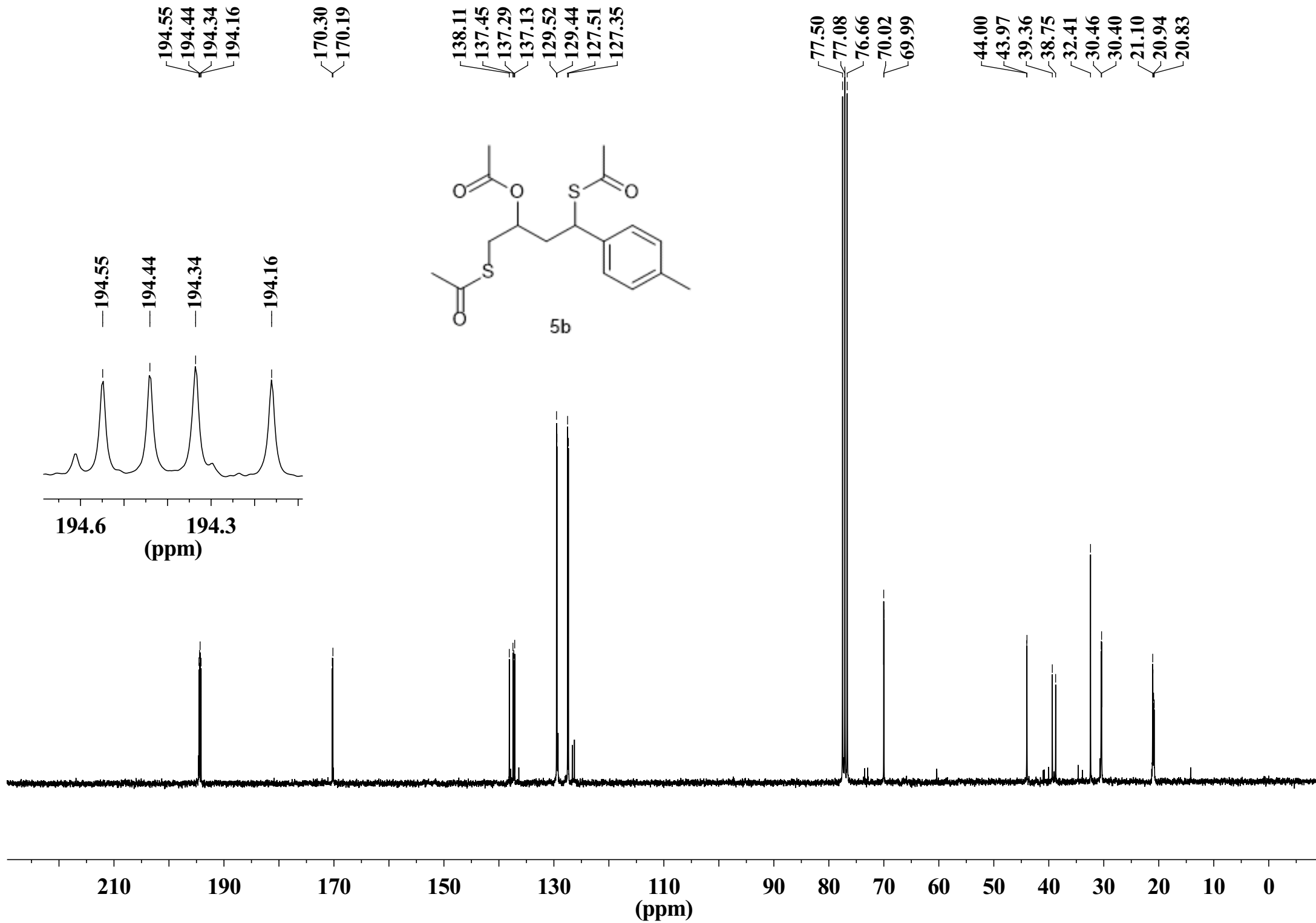
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7.19
7.19
7.17
7.17
7.15
7.14
7.14
7.13
7.11
7.10

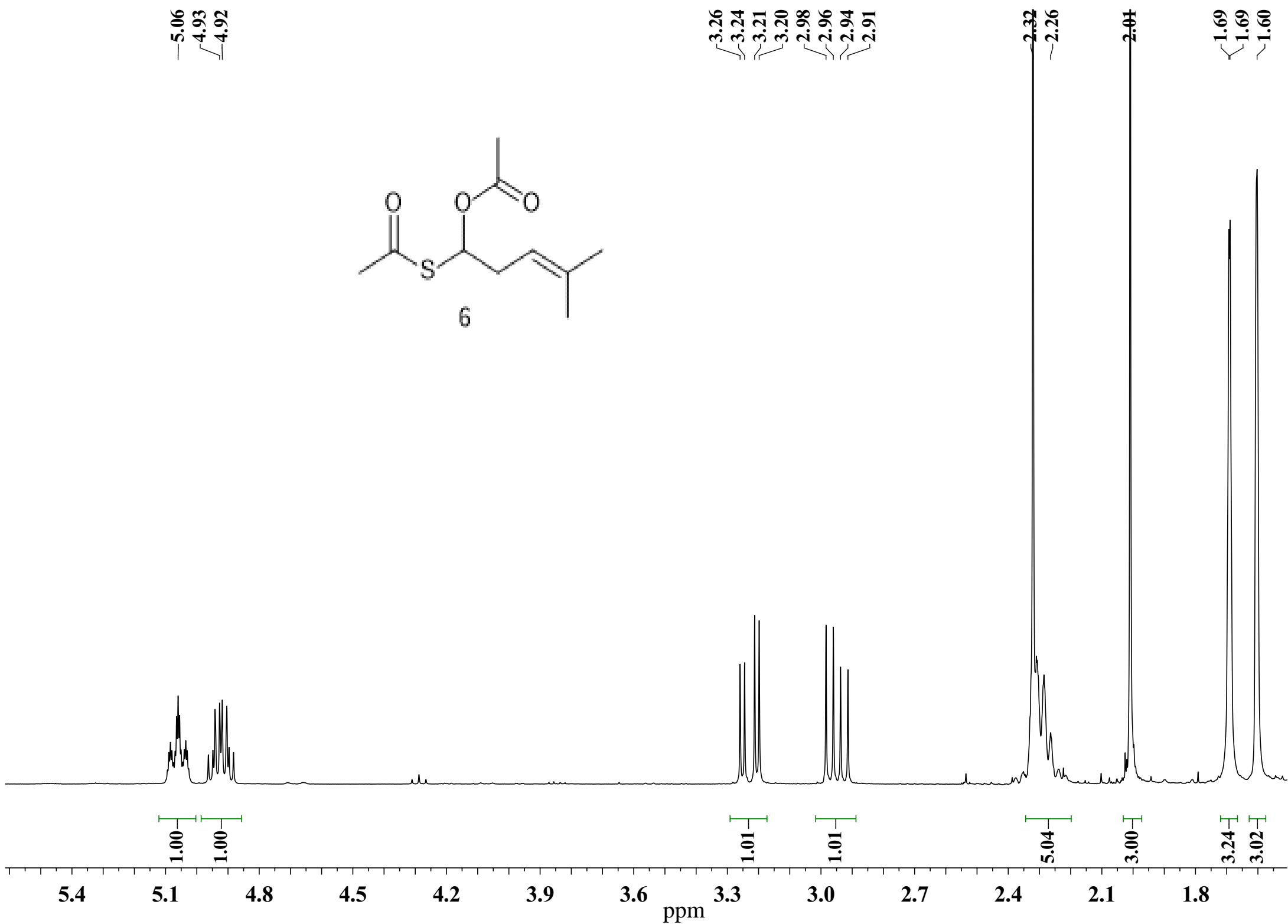
5.09
5.08
5.06
5.05

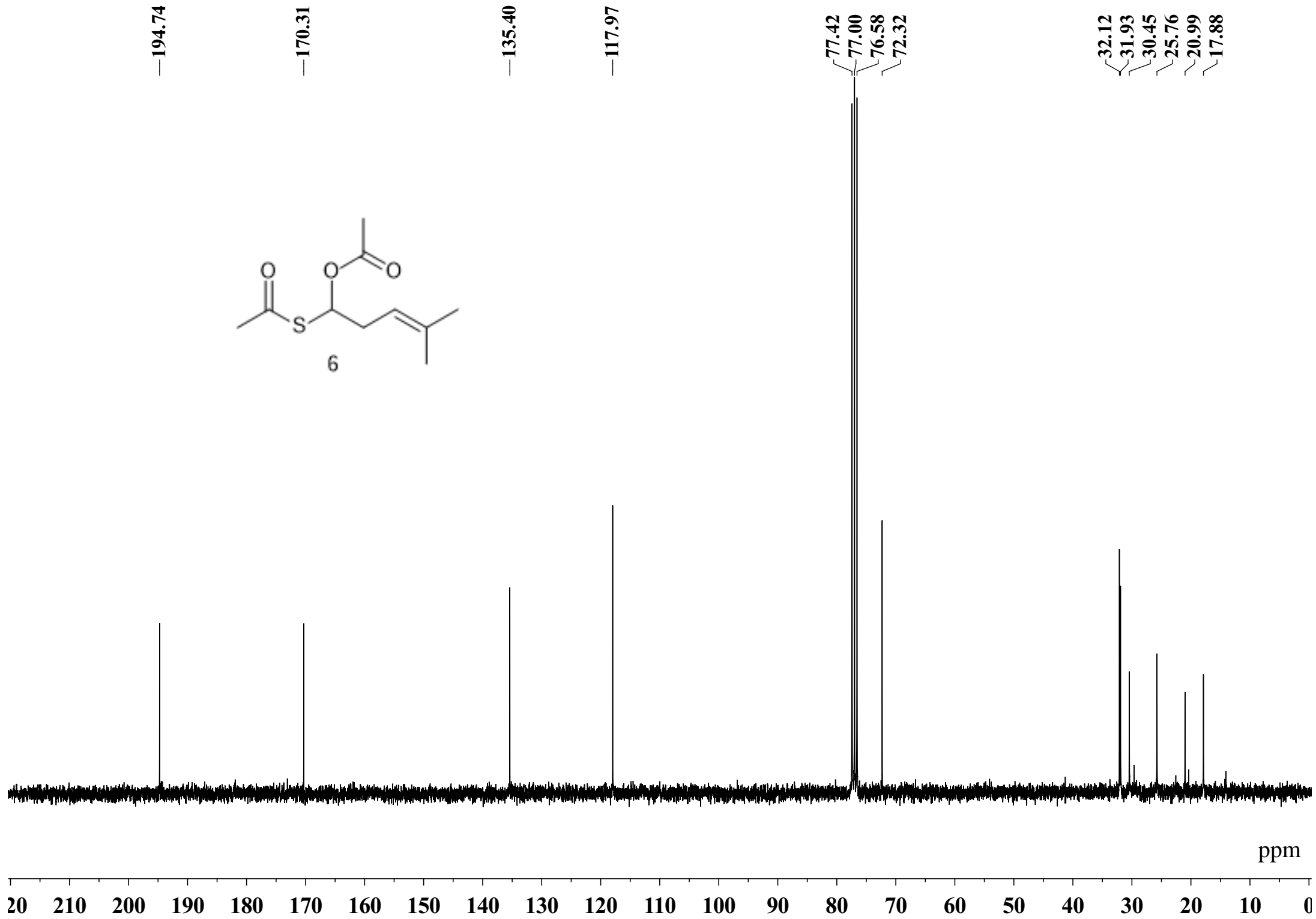
4.77
4.68
4.66
4.65
4.63
4.62
4.60
4.59
4.57

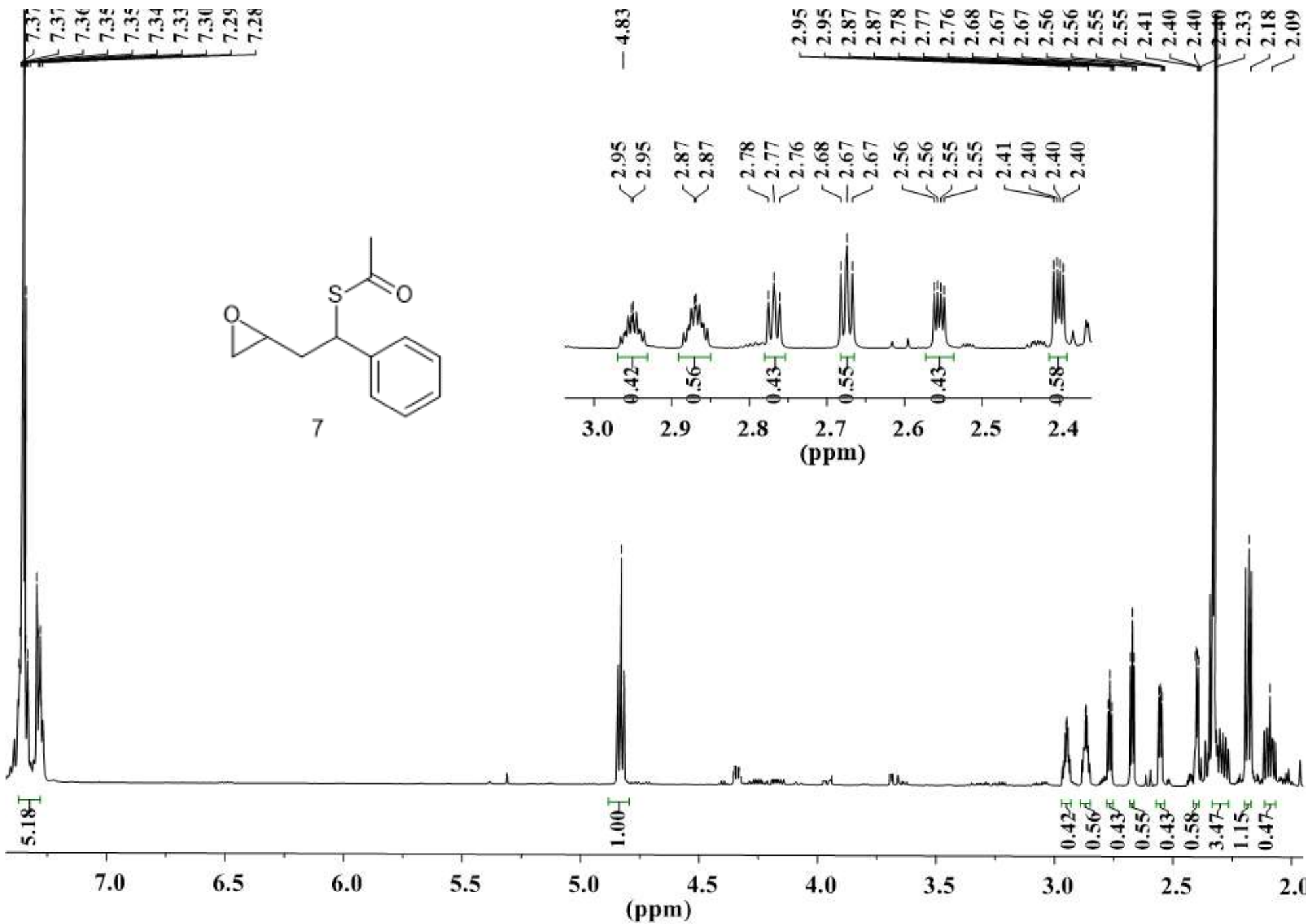
3.25
3.24
3.21
3.19
3.07
3.05
3.02
3.02
3.00
3.00
2.98
2.96
2.34
2.32
2.30
2.28
2.27
2.03
1.94









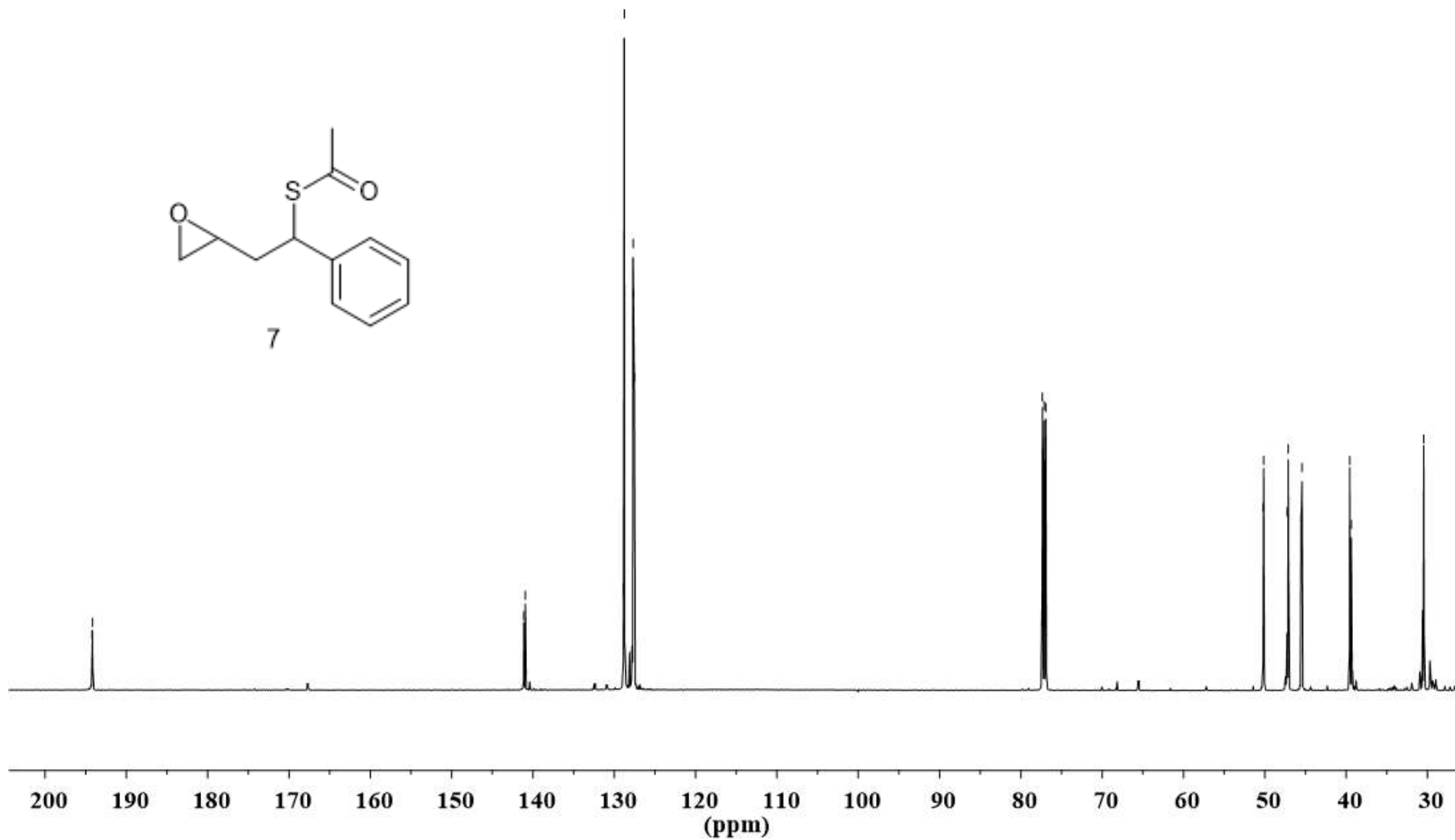
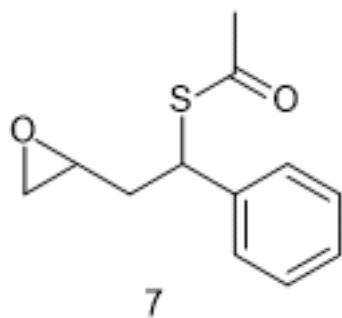


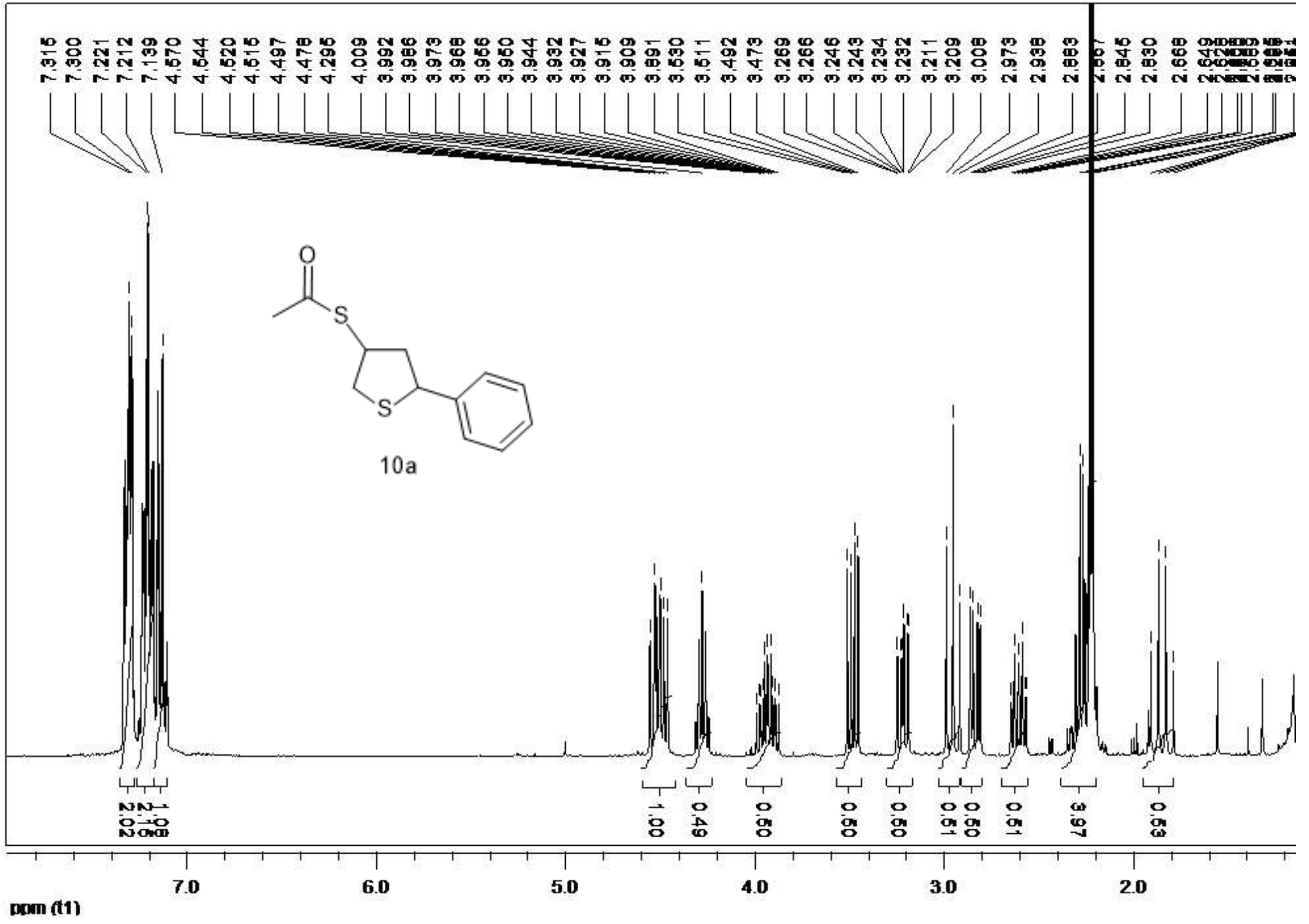
194.22
194.16

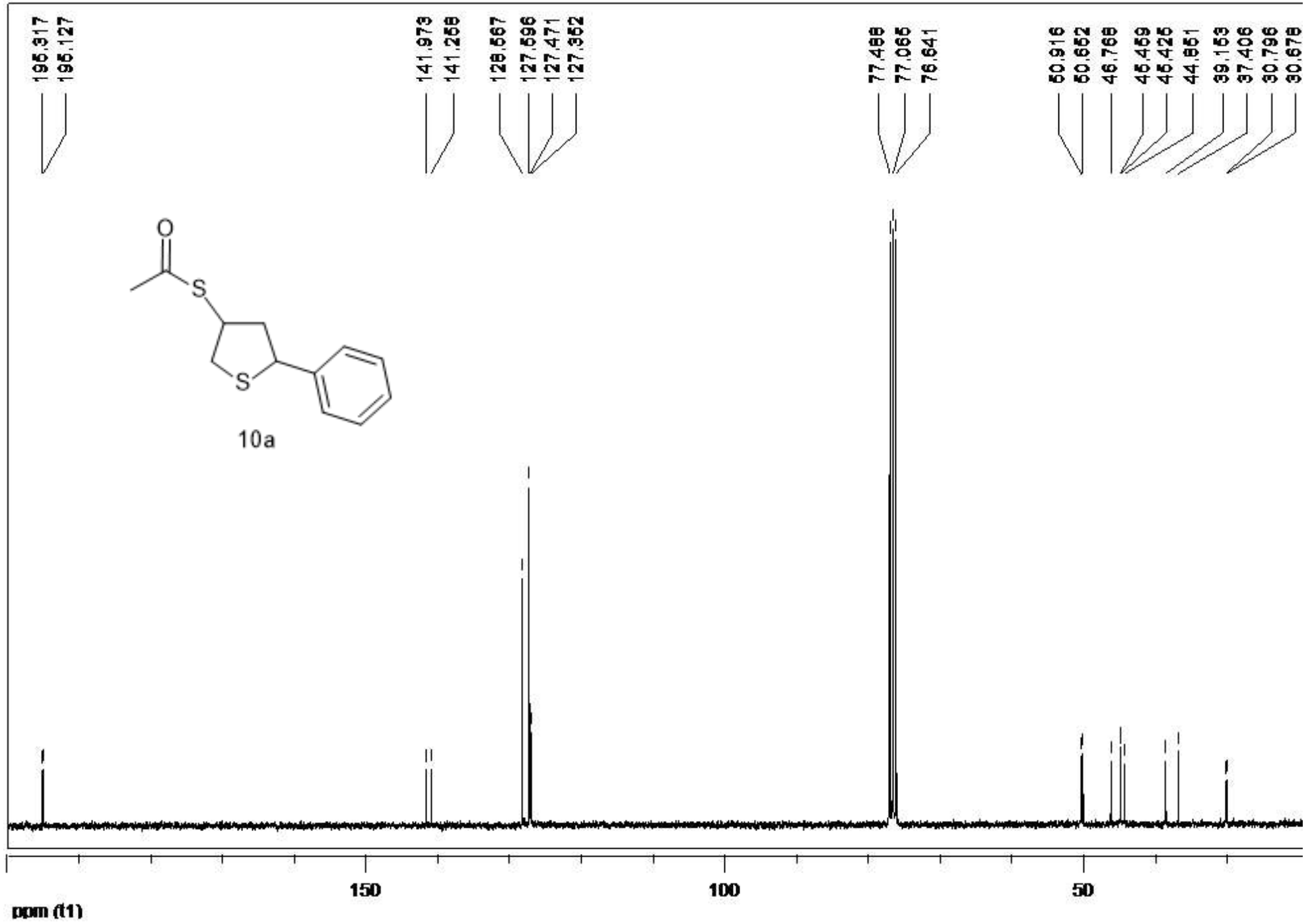
141.12
140.94
128.86
128.82
128.76
127.67
127.63
127.53

77.35
77.13
76.92

50.18
50.14
47.25
47.11
45.54
45.43
39.56
39.37
30.45







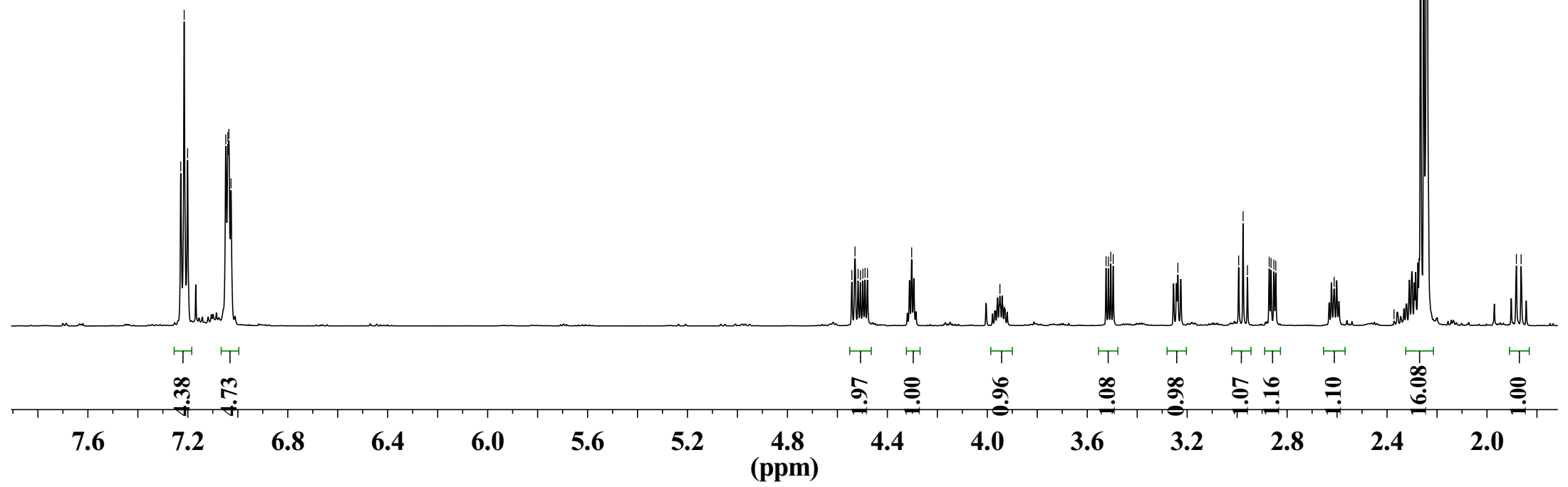
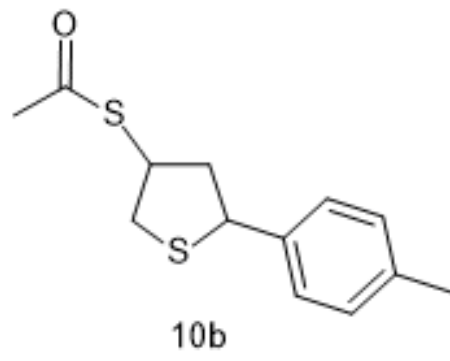
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7.21
7.20
7.05
7.04
7.04
7.03

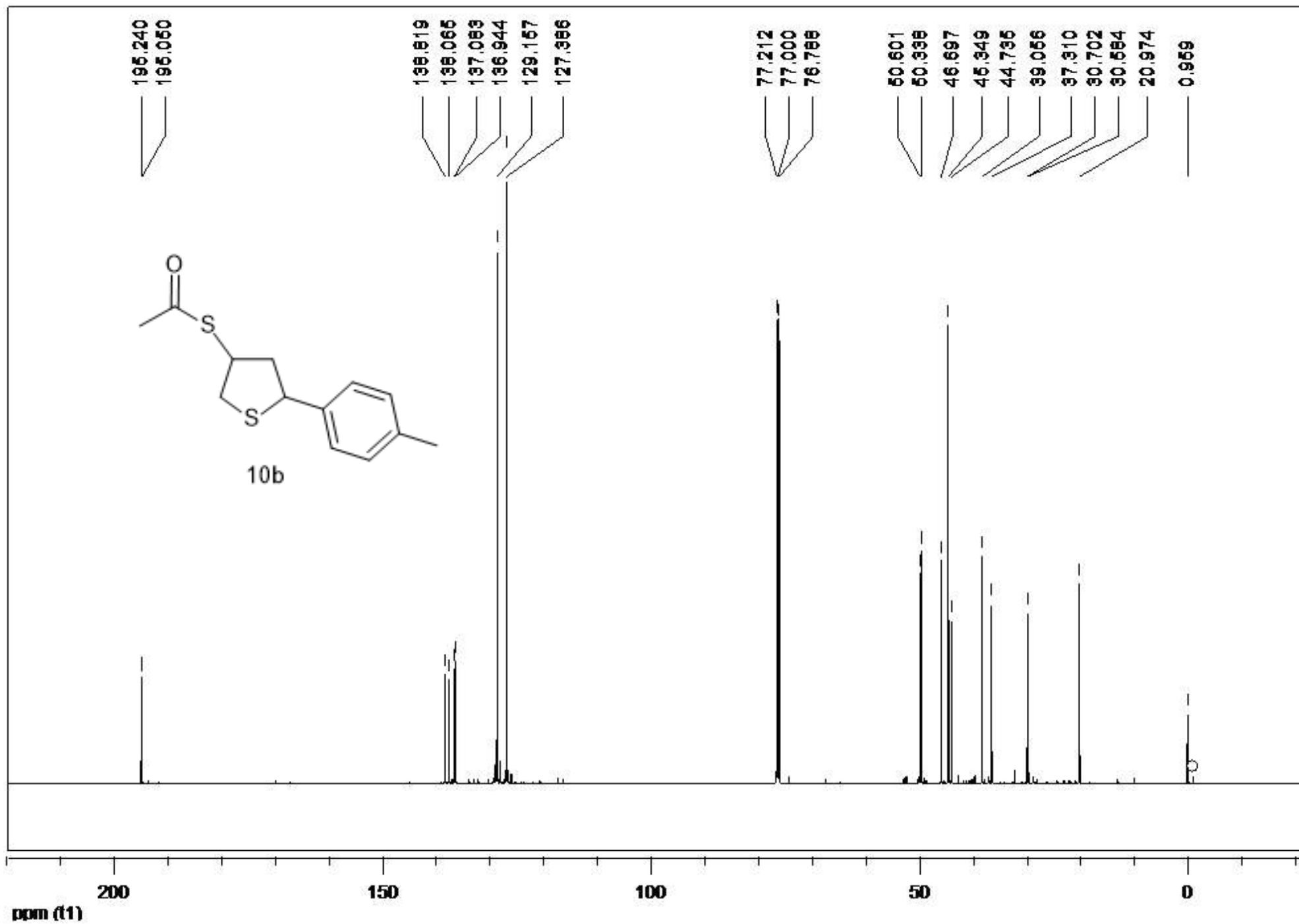
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4.53
4.52
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4.50
4.49
4.48
4.30
3.95

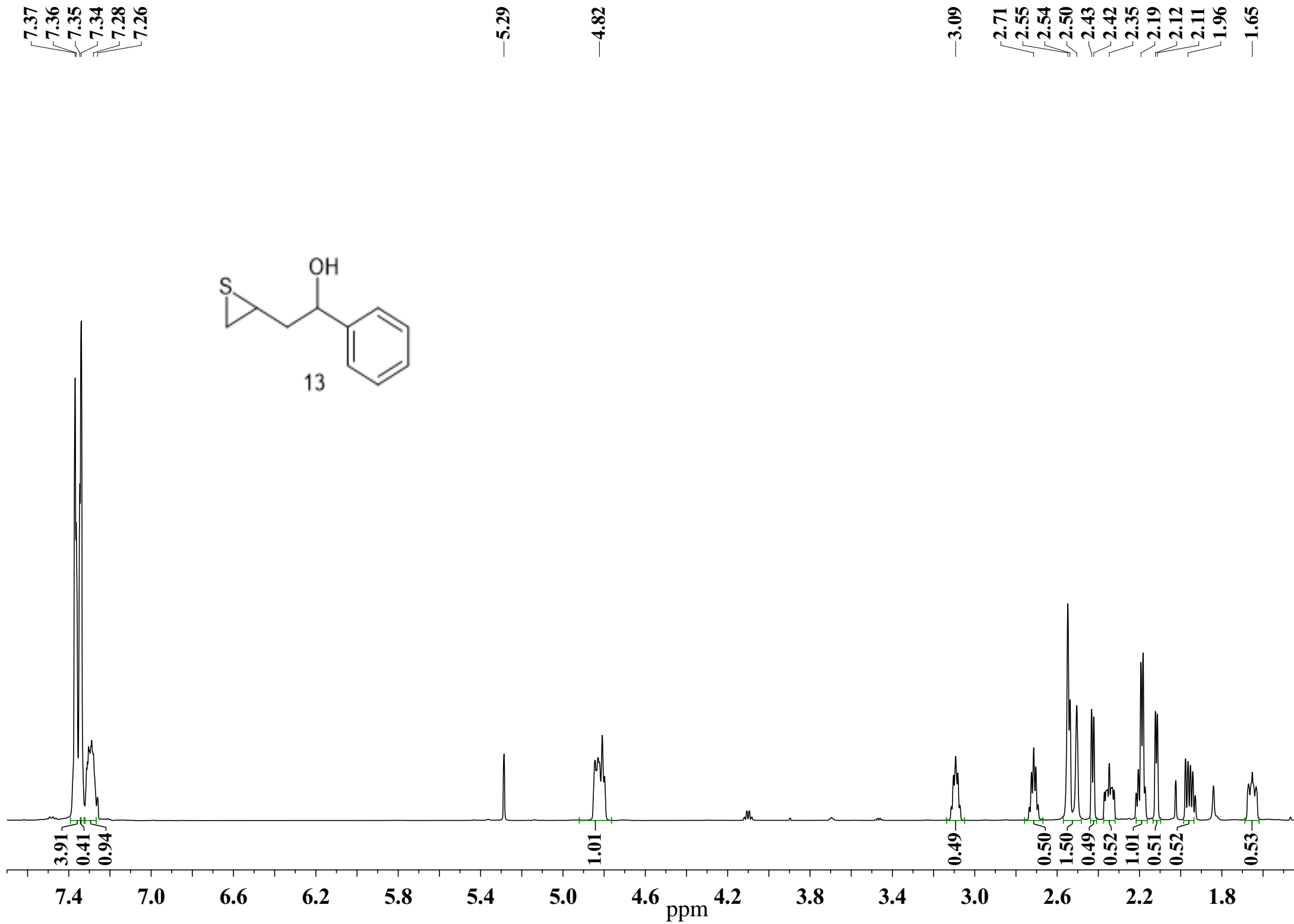
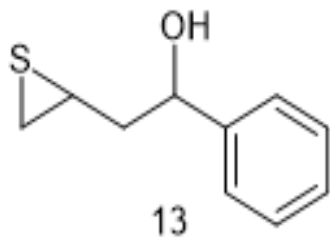
3.52
3.52
3.51
3.50
3.24

2.99
2.98
2.87
2.86
2.61
2.37
2.27
2.25
2.24

1.88
1.86







144.09
143.62

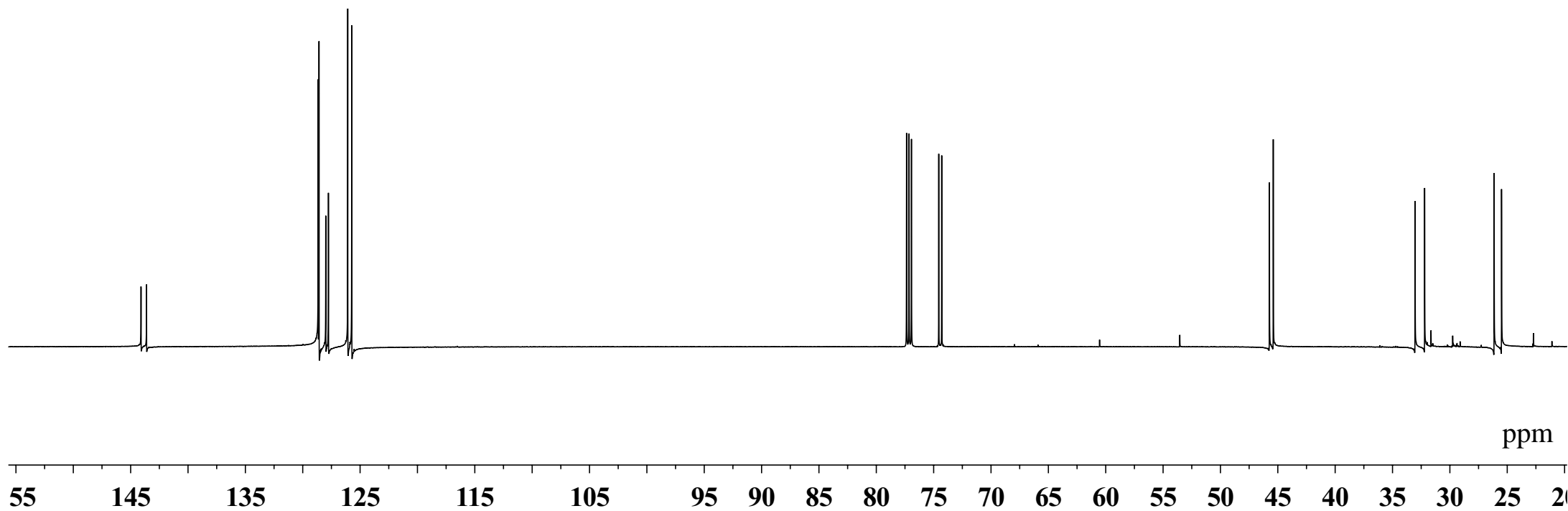
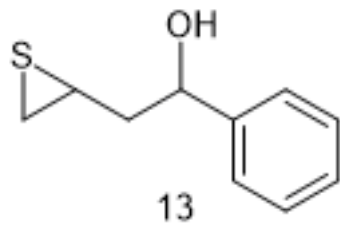
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128.58
127.99
127.76
126.08
125.73

77.36
77.15
76.94
74.56
74.30

45.73
45.40

33.03
32.20

26.14
25.50

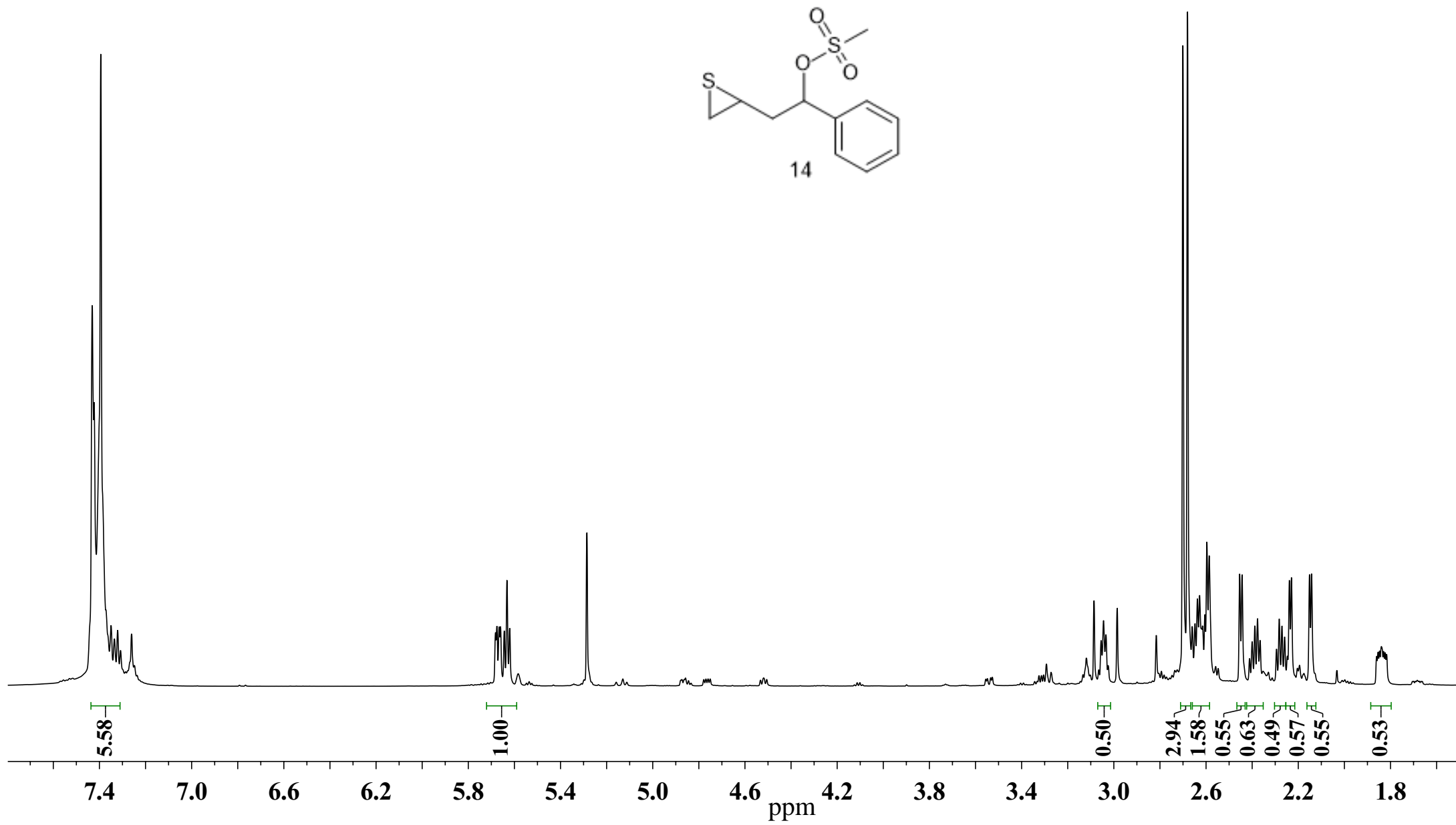
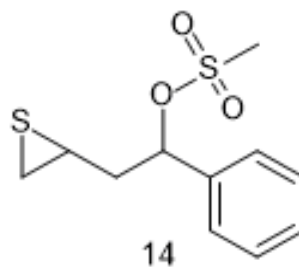


7.43
7.31

5.68
5.63

5.29

3.04
2.70
2.68
2.66
2.59
2.45
2.44
2.24
2.23
2.15
1.84



137.66
137.09
129.42
129.25
129.00
128.93
126.81
126.48

84.60
83.88
77.21
77.00
76.79

44.09
43.39
38.97

31.42
30.35
25.91
25.20

