

Supporting Information: Spectra Data

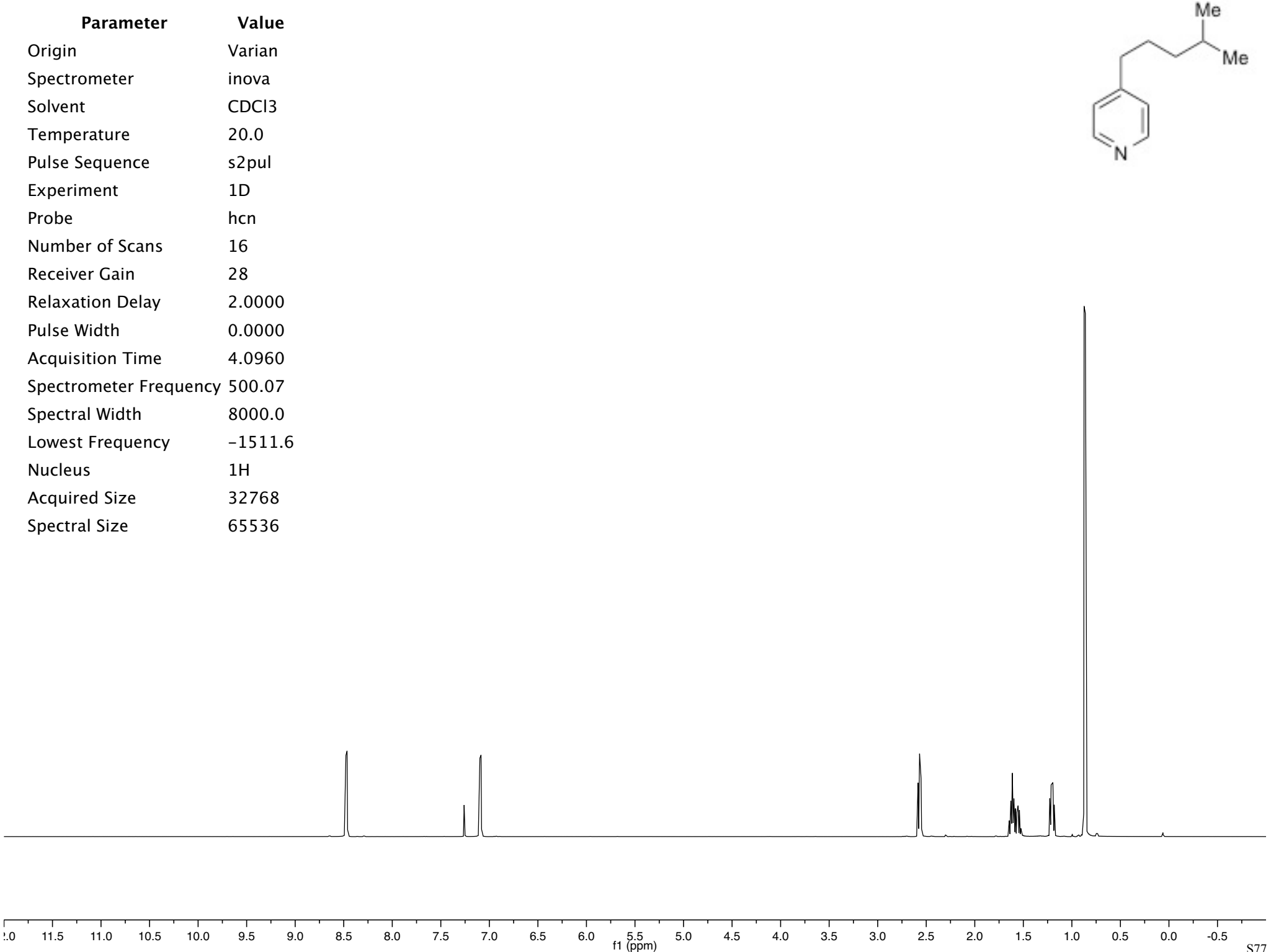
Remote Oxidation of Aliphatic C—H Bonds in Nitrogen-Containing Molecules

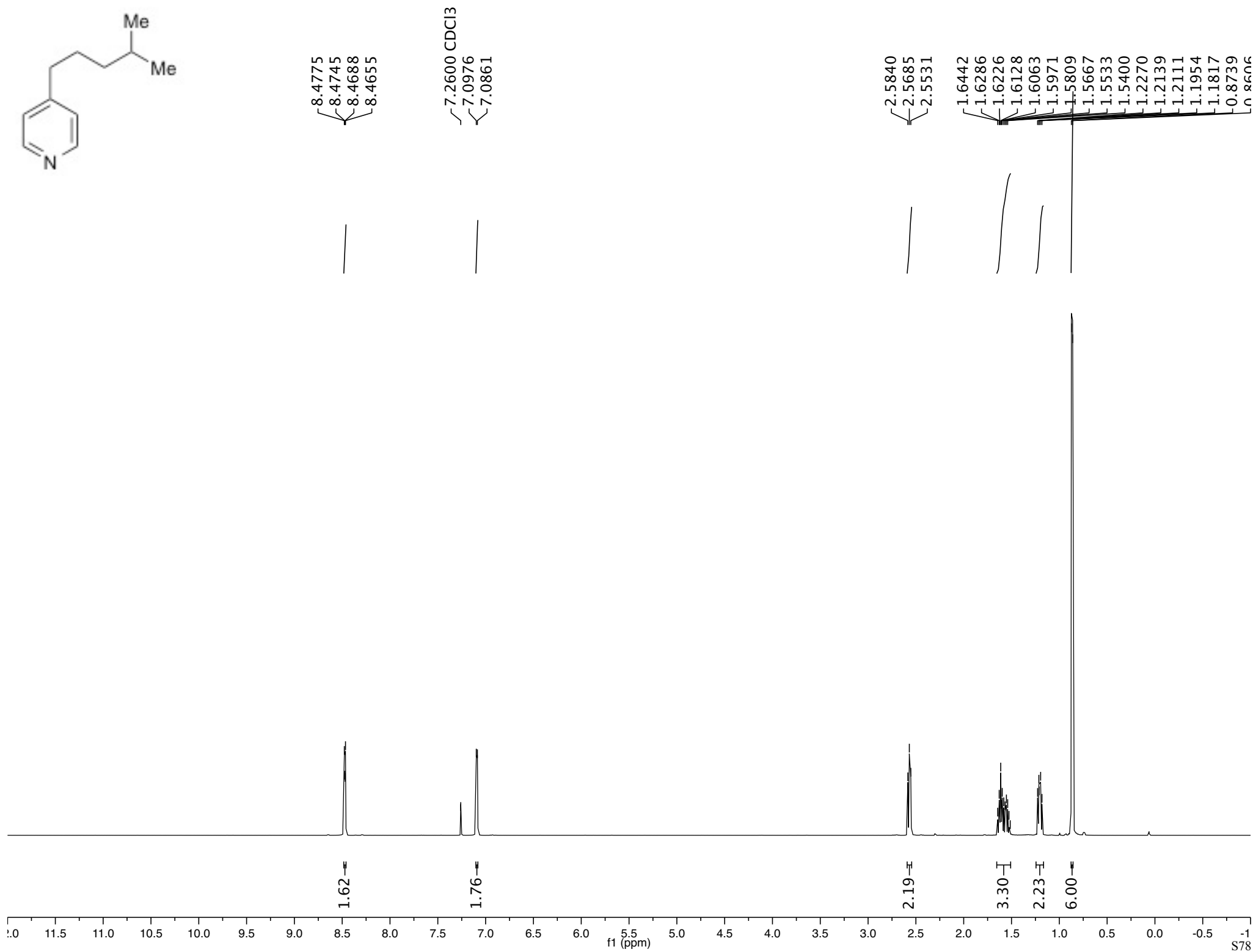
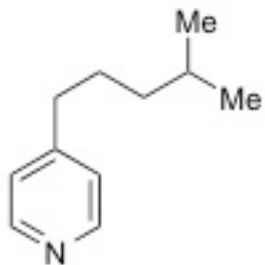
Jennifer M. Howell[‡], Kaibo Feng[‡], Joseph R. Clark, Louis J. Trzepkowski and M. Christina White*

Roger Adams Laboratory, Department of Chemistry, University of Illinois, Urbana, Illinois 61801, United States

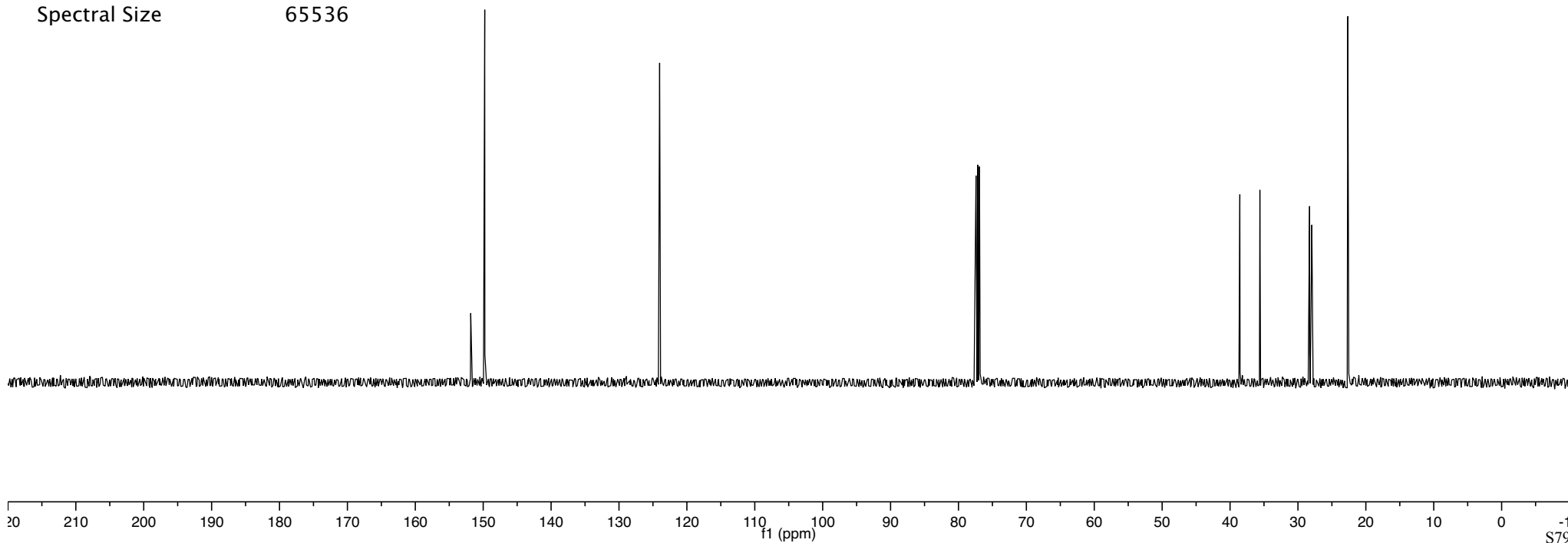
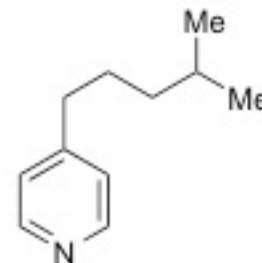
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	28
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1511.6
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

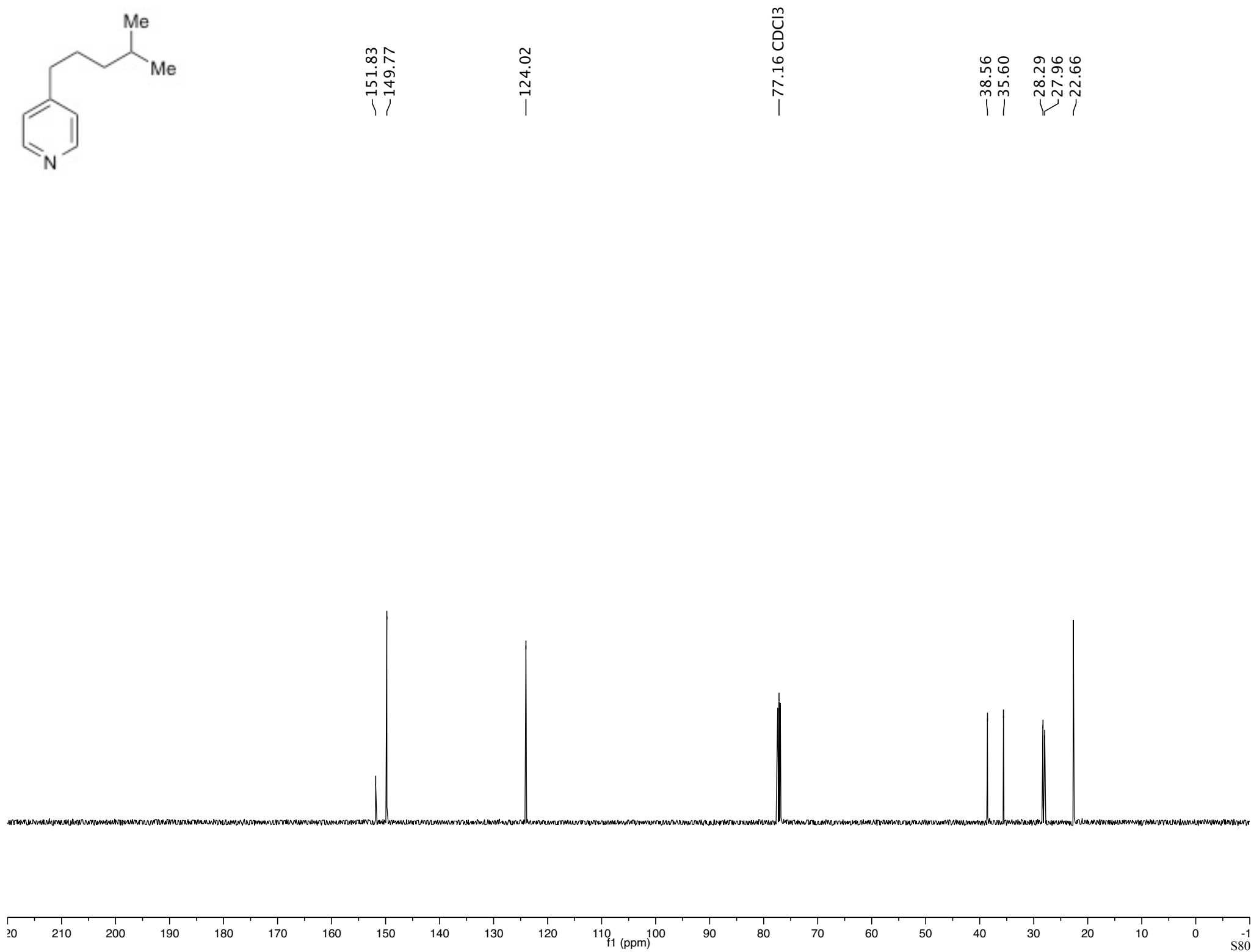
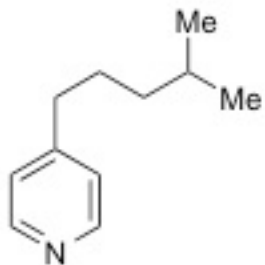
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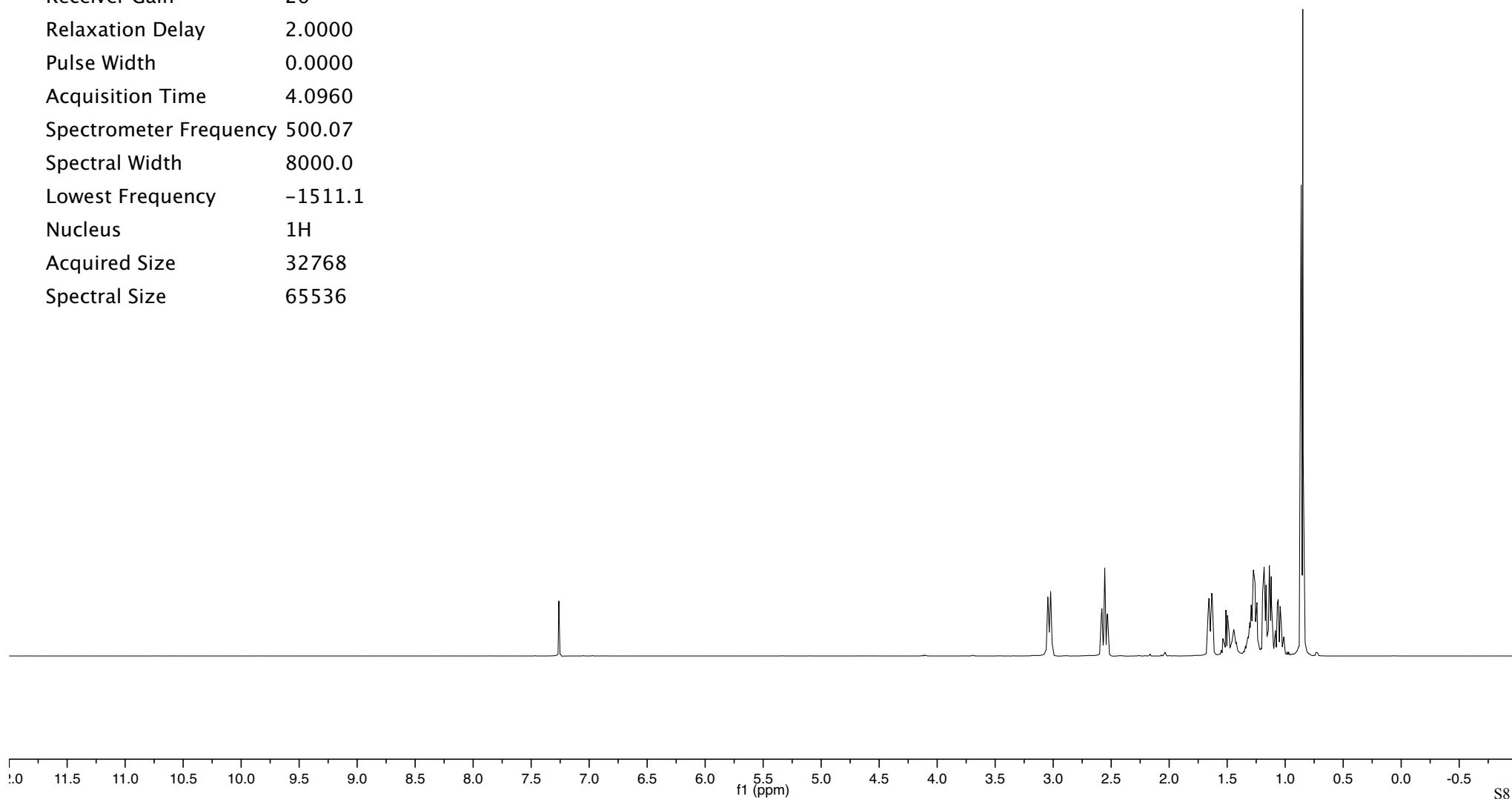
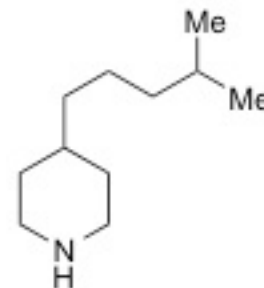


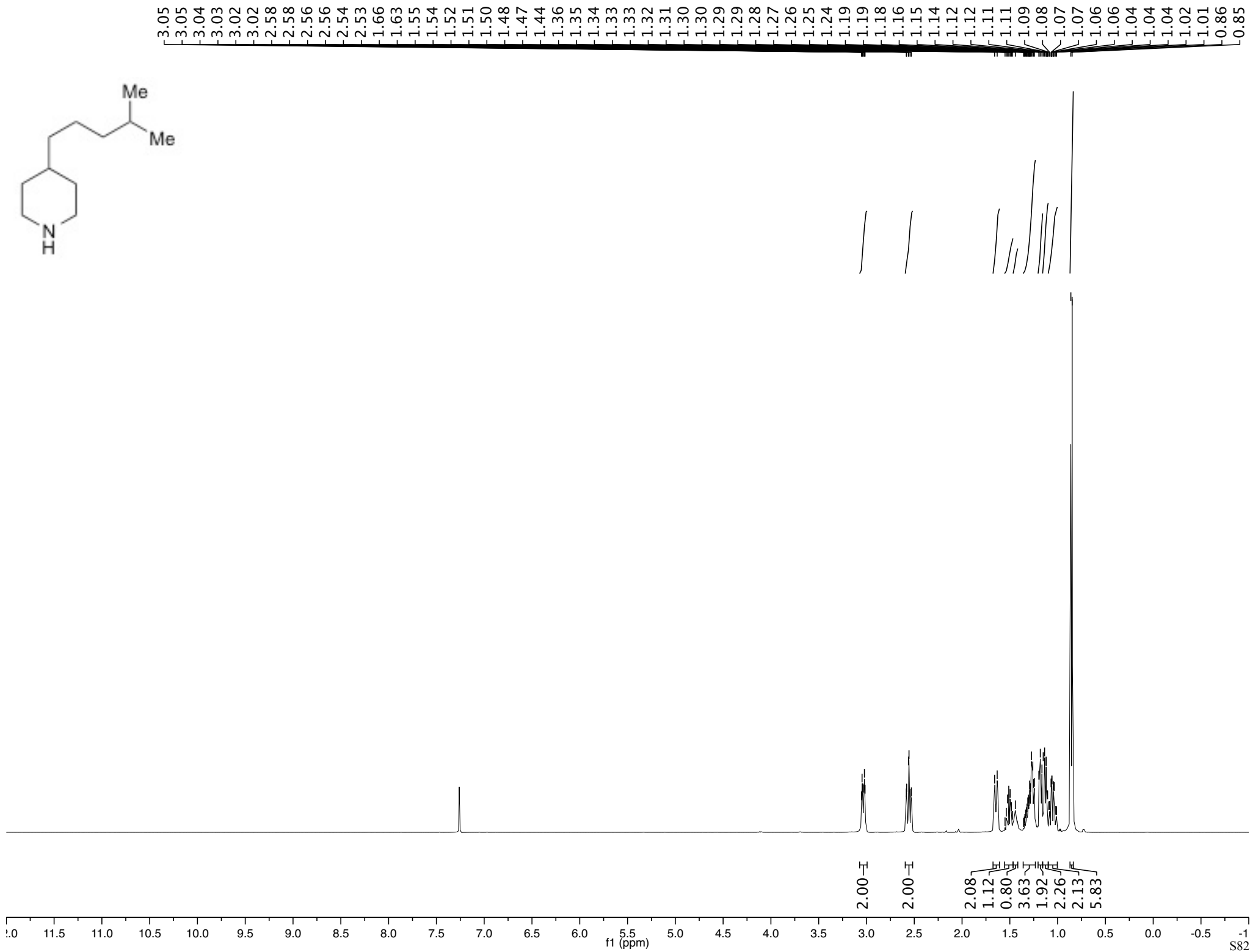
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Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	176
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1271.6
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



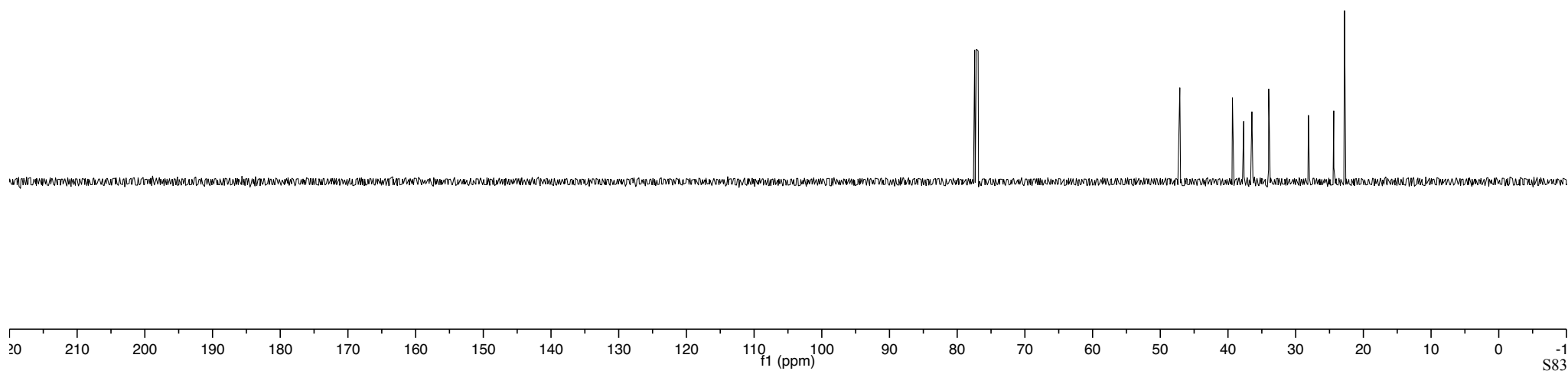
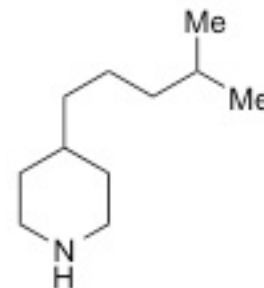


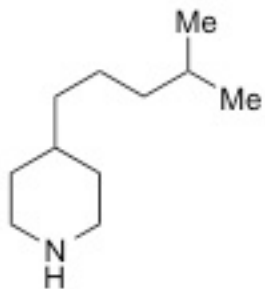
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Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	26
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1511.1
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536





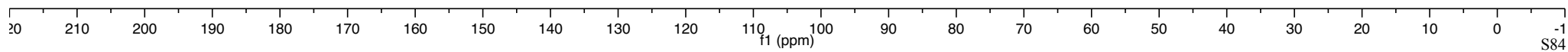
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Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	96
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1271.1
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



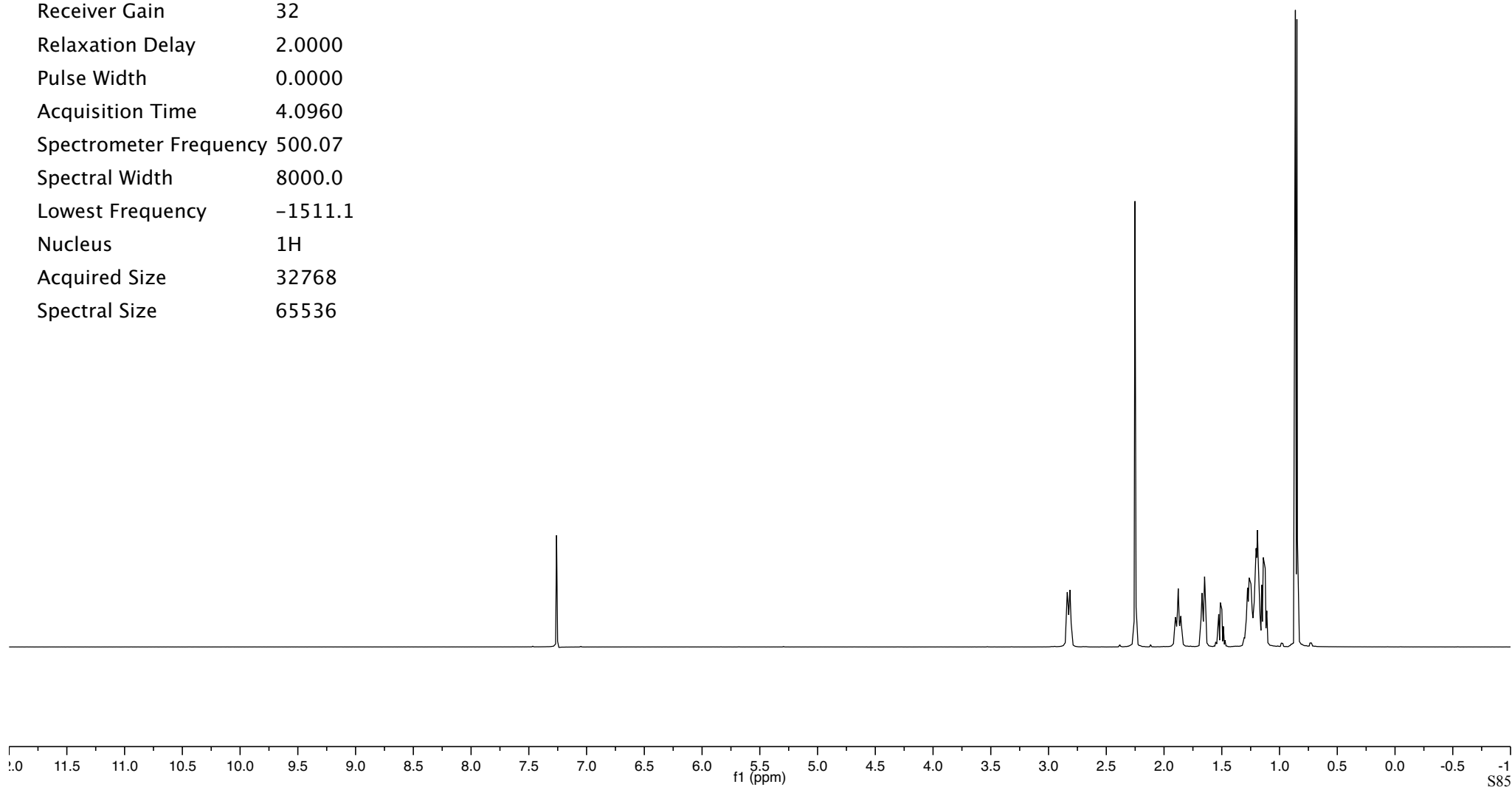
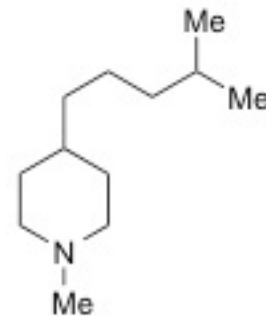


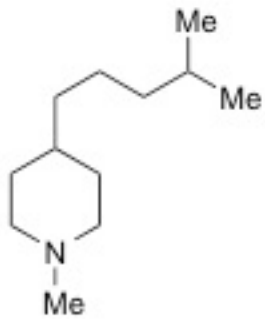
—77.16 CDCl₃

—47.11
—39.34
—37.68
—36.47
—33.98
—28.11
—24.38
—22.78

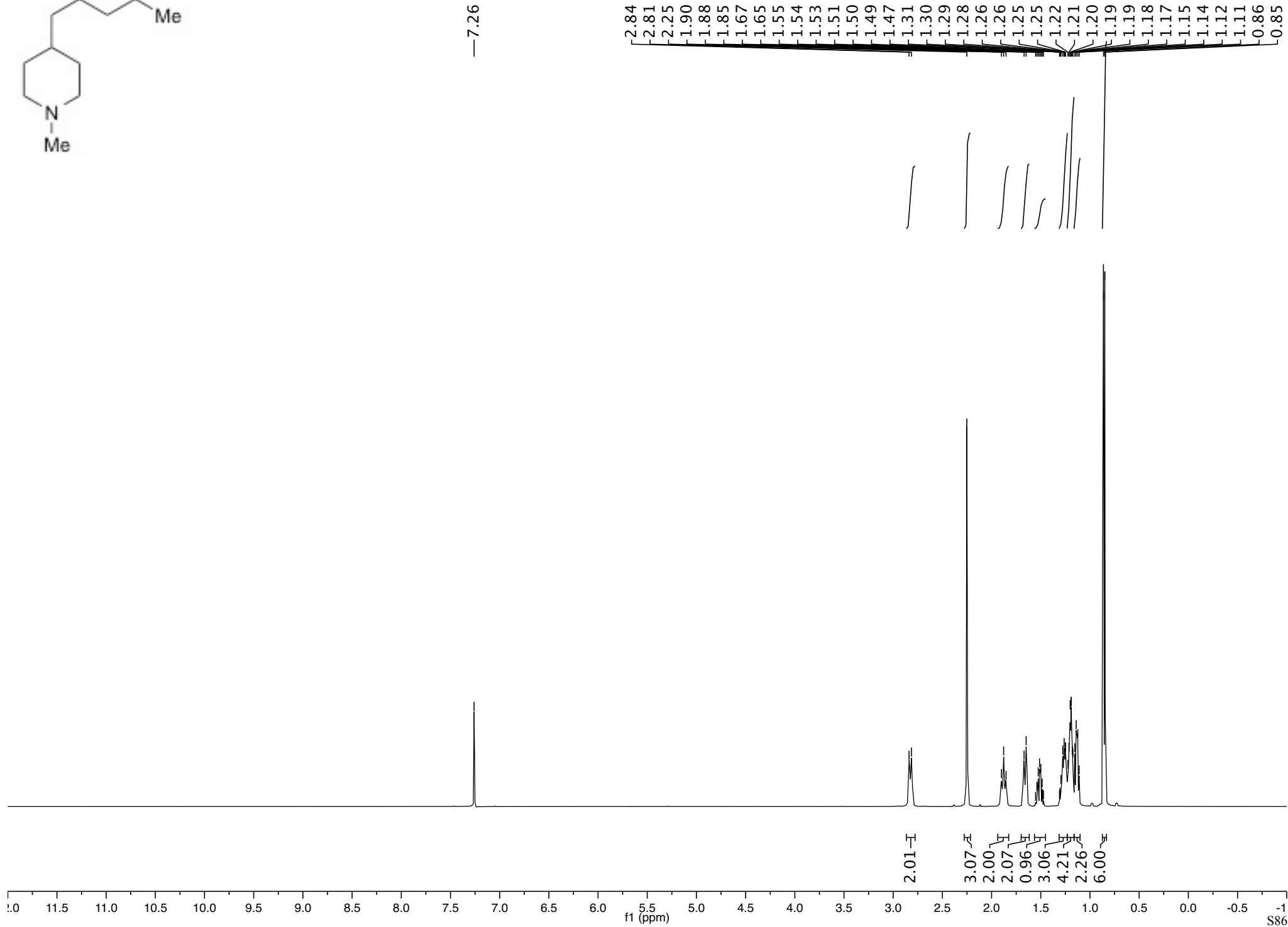


Parameter	Value
Title	JMH-III-32_1H
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	32
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1511.1
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

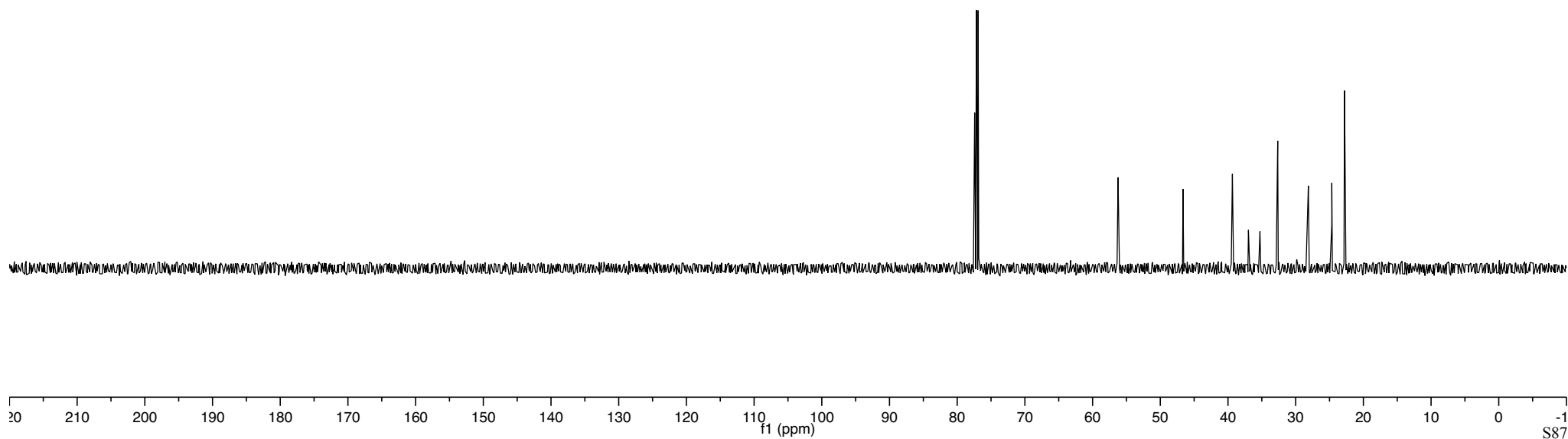
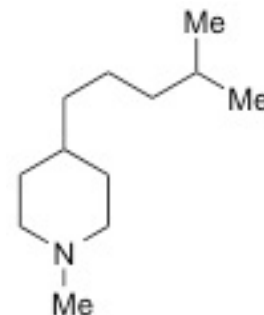


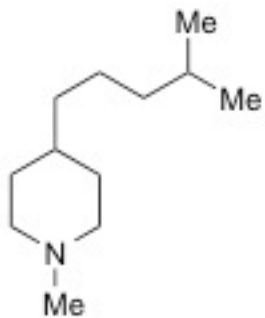


— 7.26 CDCl₃



Parameter	Value
Title	JMH-III-22_13C
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	192
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1270.2
Nucleus	13C
Acquired Size	32768
Spectral Size	65536





—77.16 CDCl₃

—56.24

—46.64

—39.35

—36.98

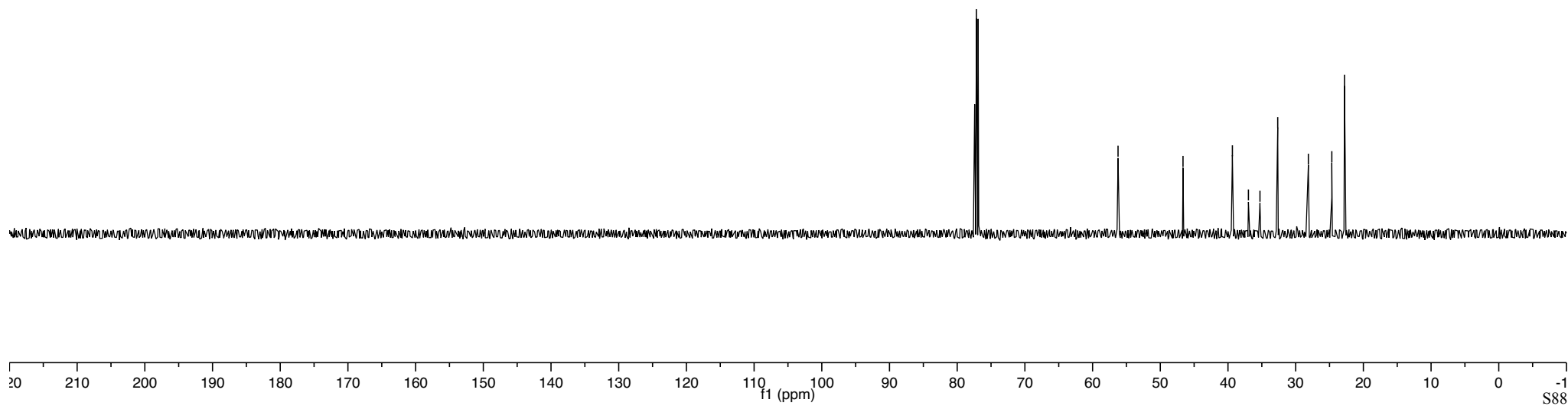
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—32.65

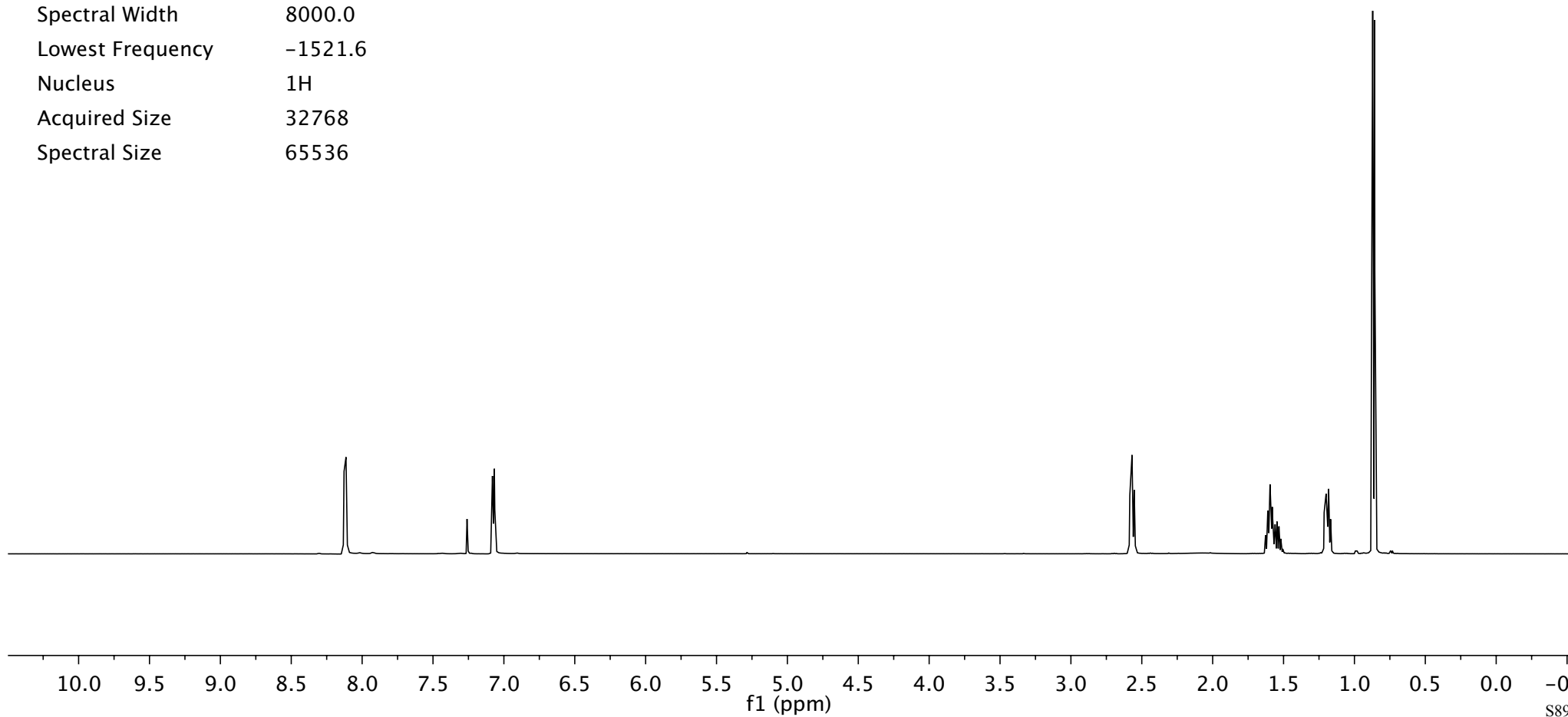
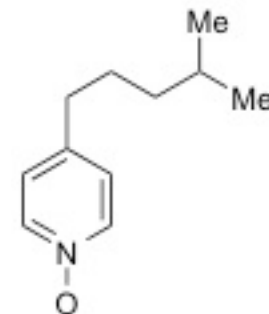
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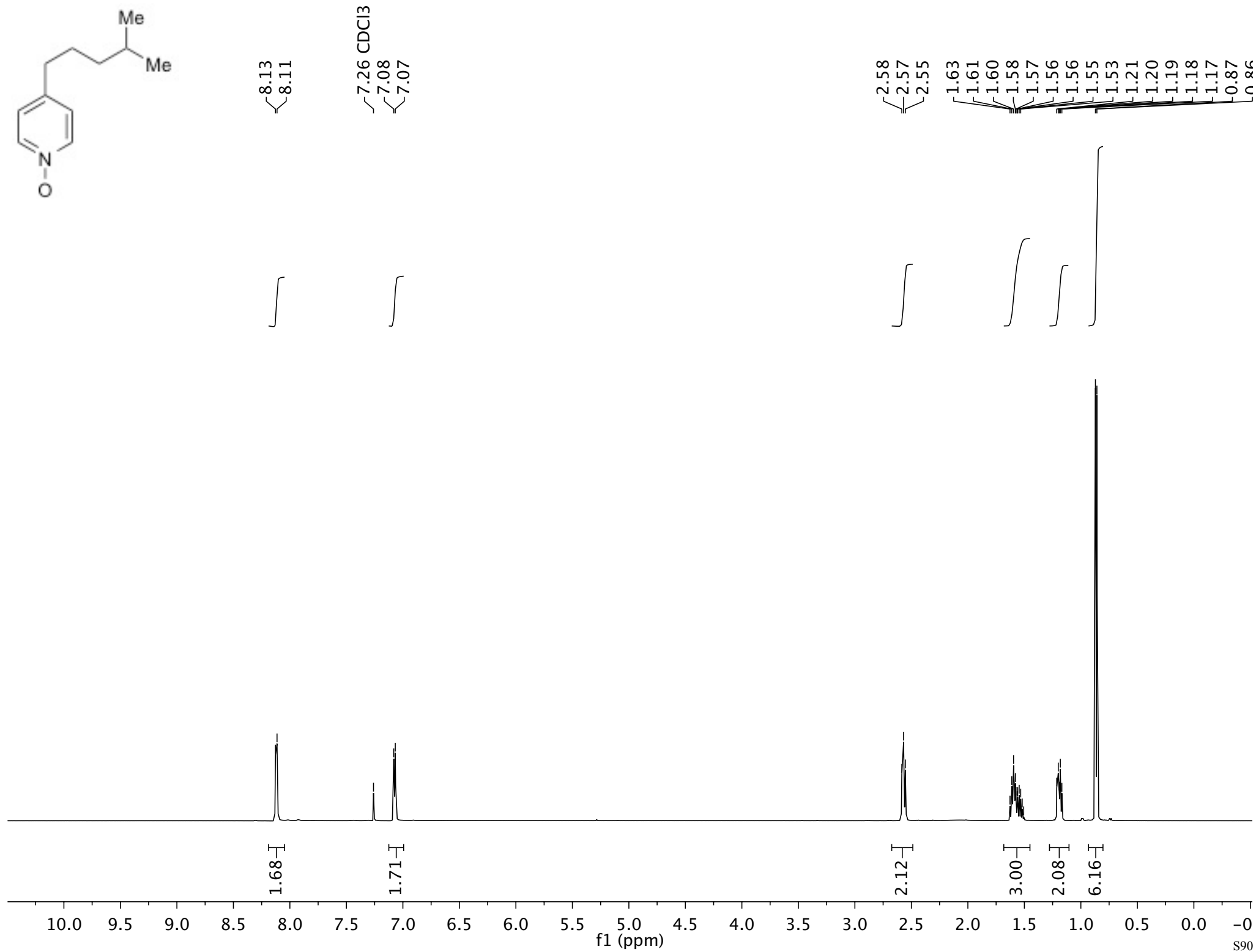
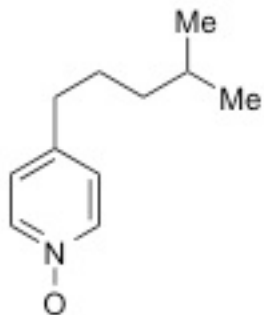
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—22.79

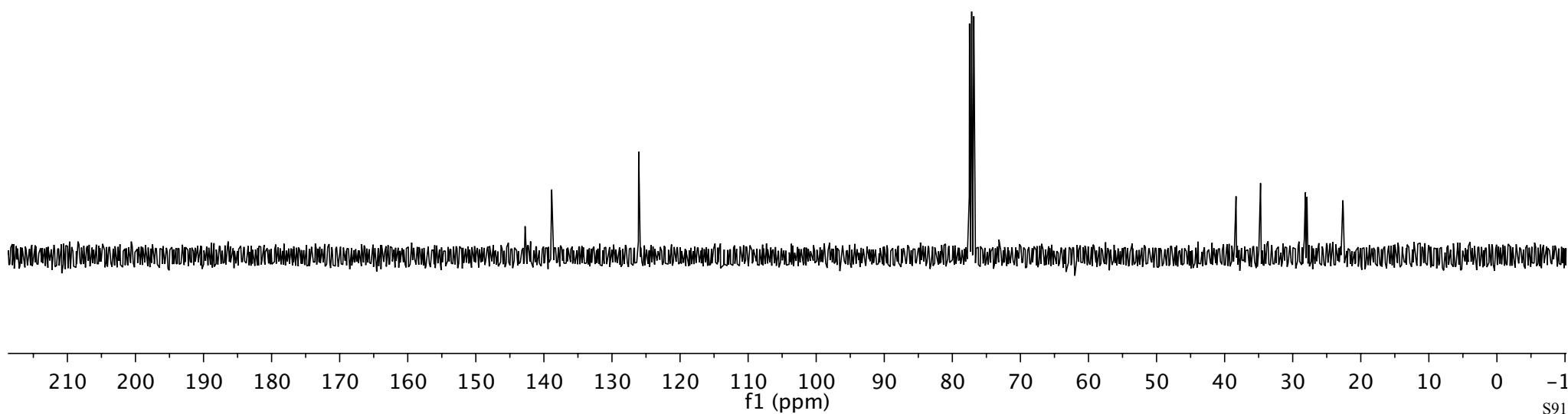
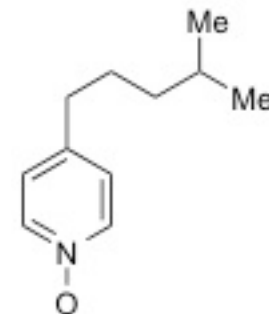


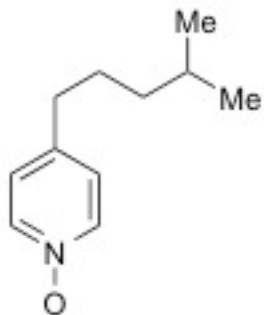
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	32
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.6
Nucleus	1H
Acquired Size	32768
Spectral Size	65536





Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.3107
Spectrometer Frequency	100.58
Spectral Width	25000.0
Lowest Frequency	-1027.7
Nucleus	13C
Acquired Size	32768
Spectral Size	65536





—142.76

—138.87

—126.07

77.48 CDCl₃

77.16 CDCl₃

76.84 CDCl₃

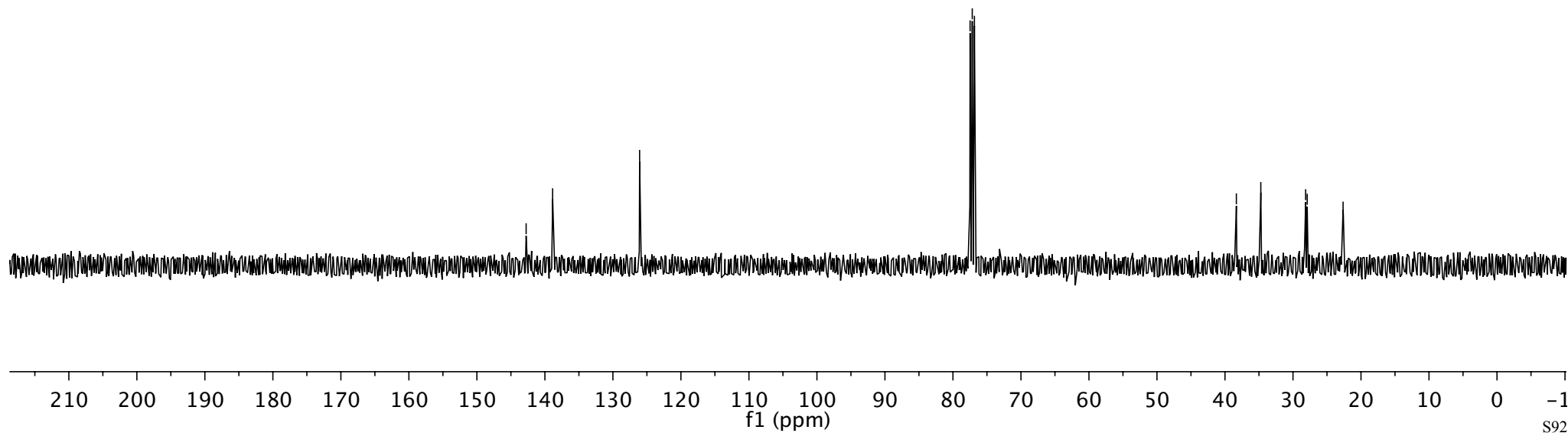
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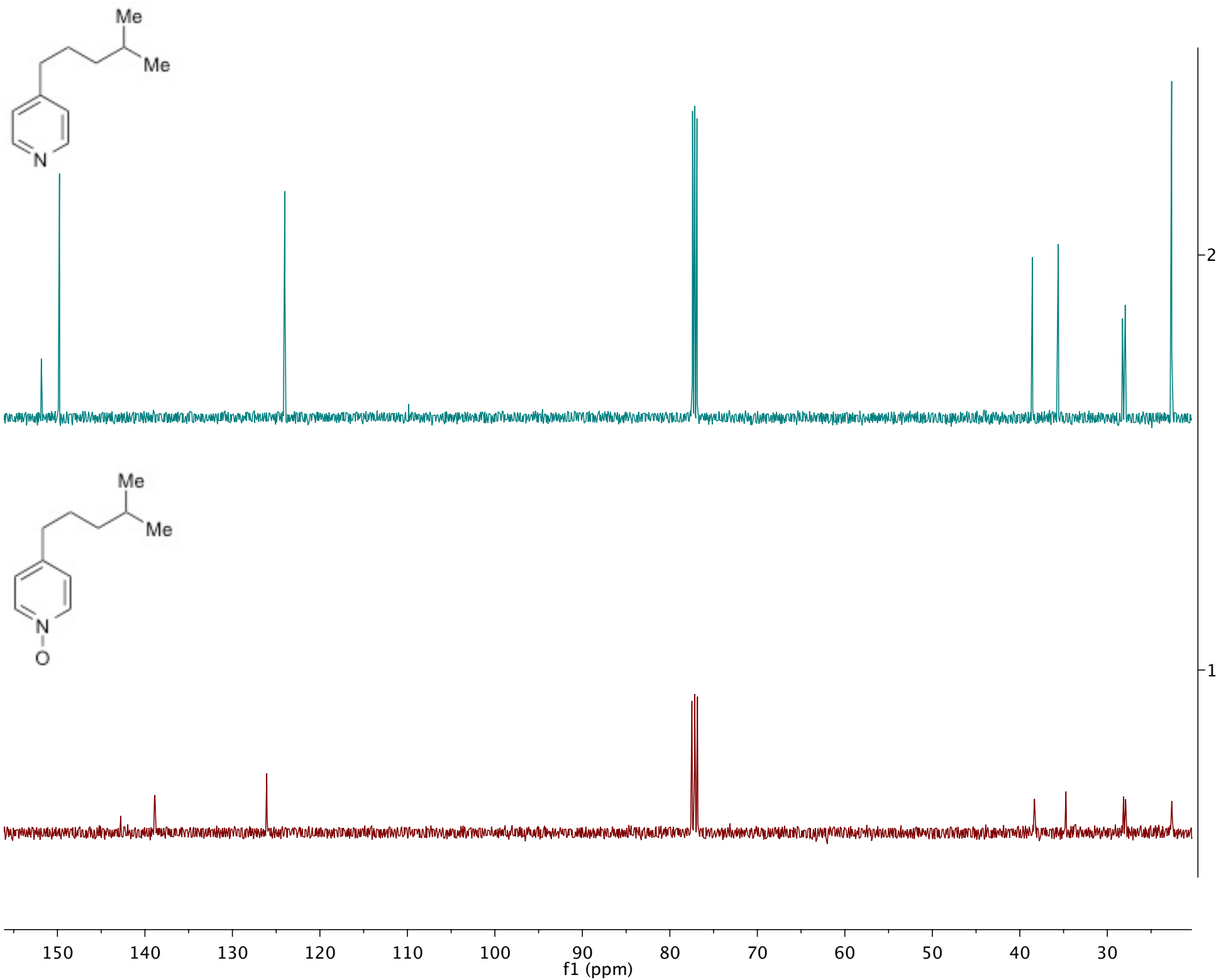
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~28.14

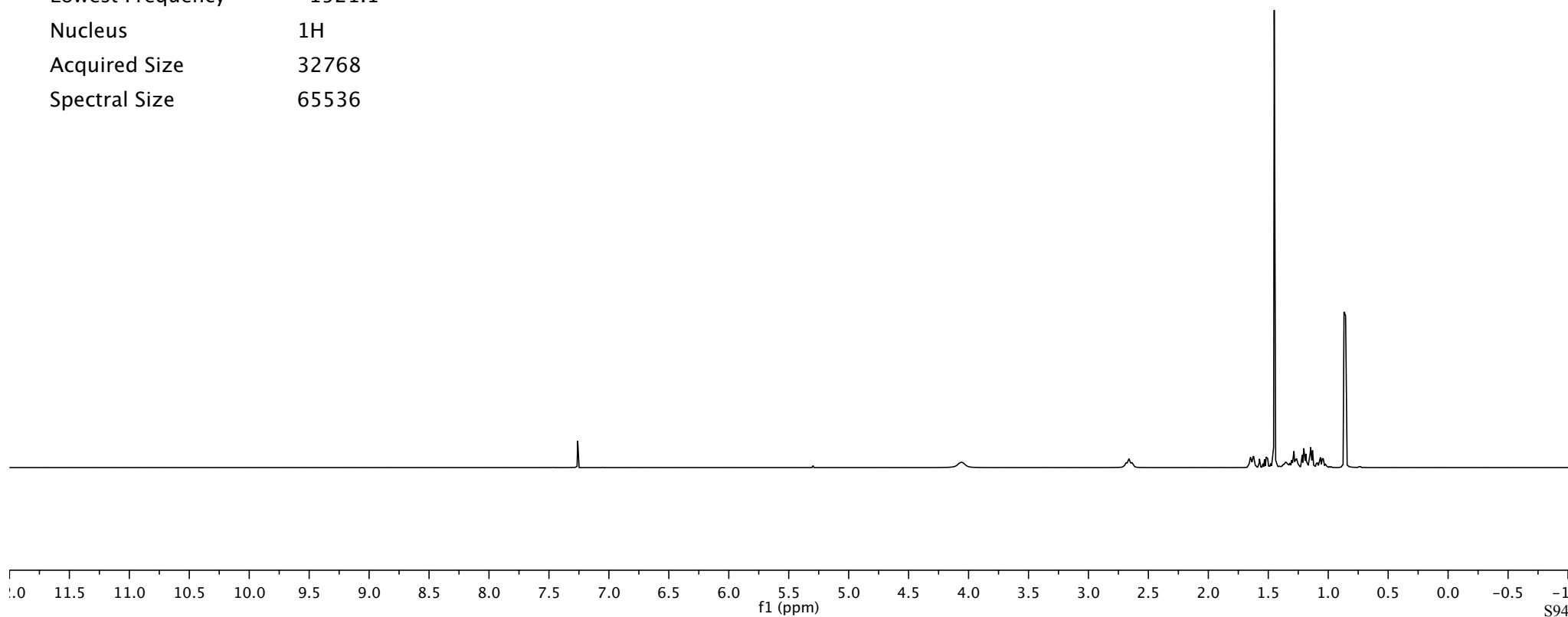
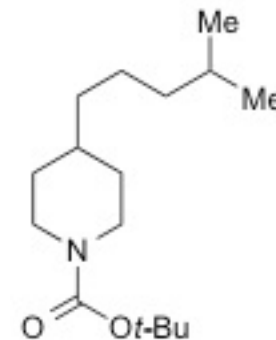
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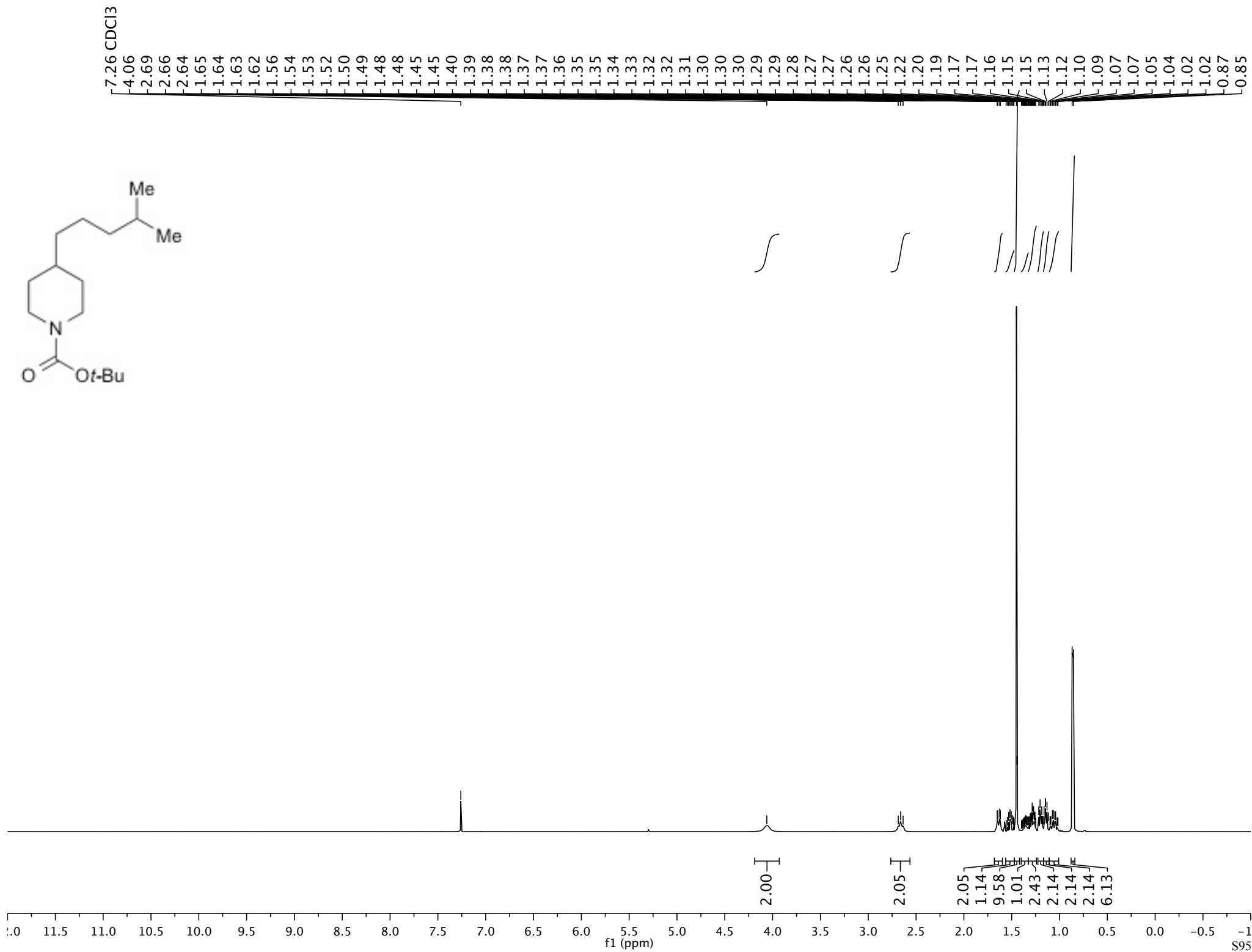
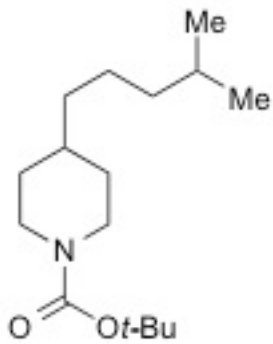
~22.63



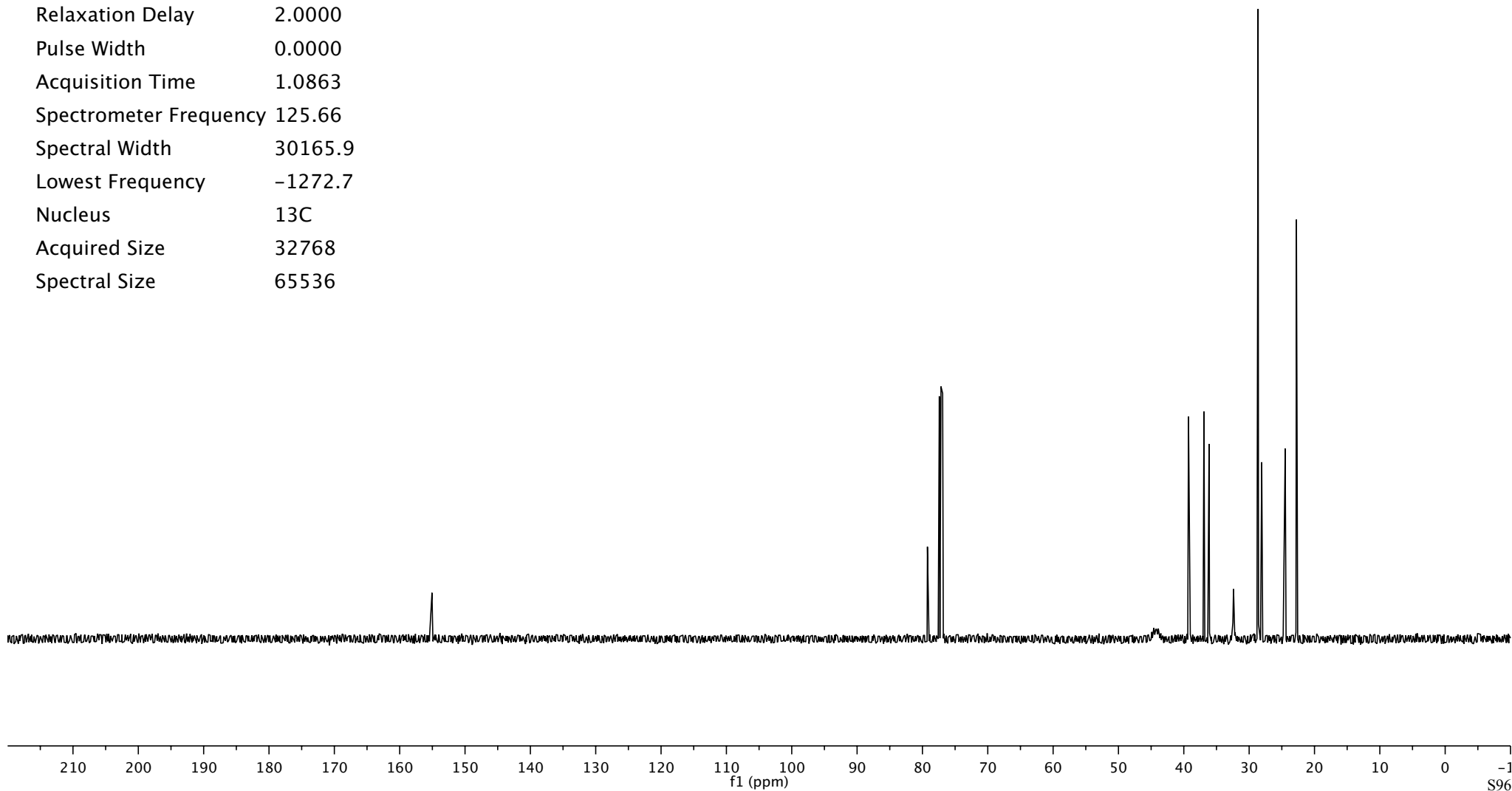
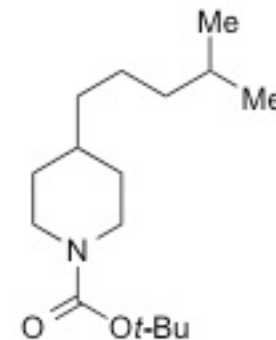


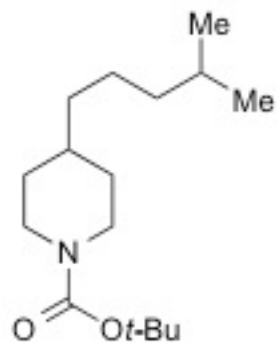
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	38
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536





Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	635
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1272.7
Nucleus	13C
Acquired Size	32768
Spectral Size	65536





—155.06

~79.23
~77.16 CDCl₃

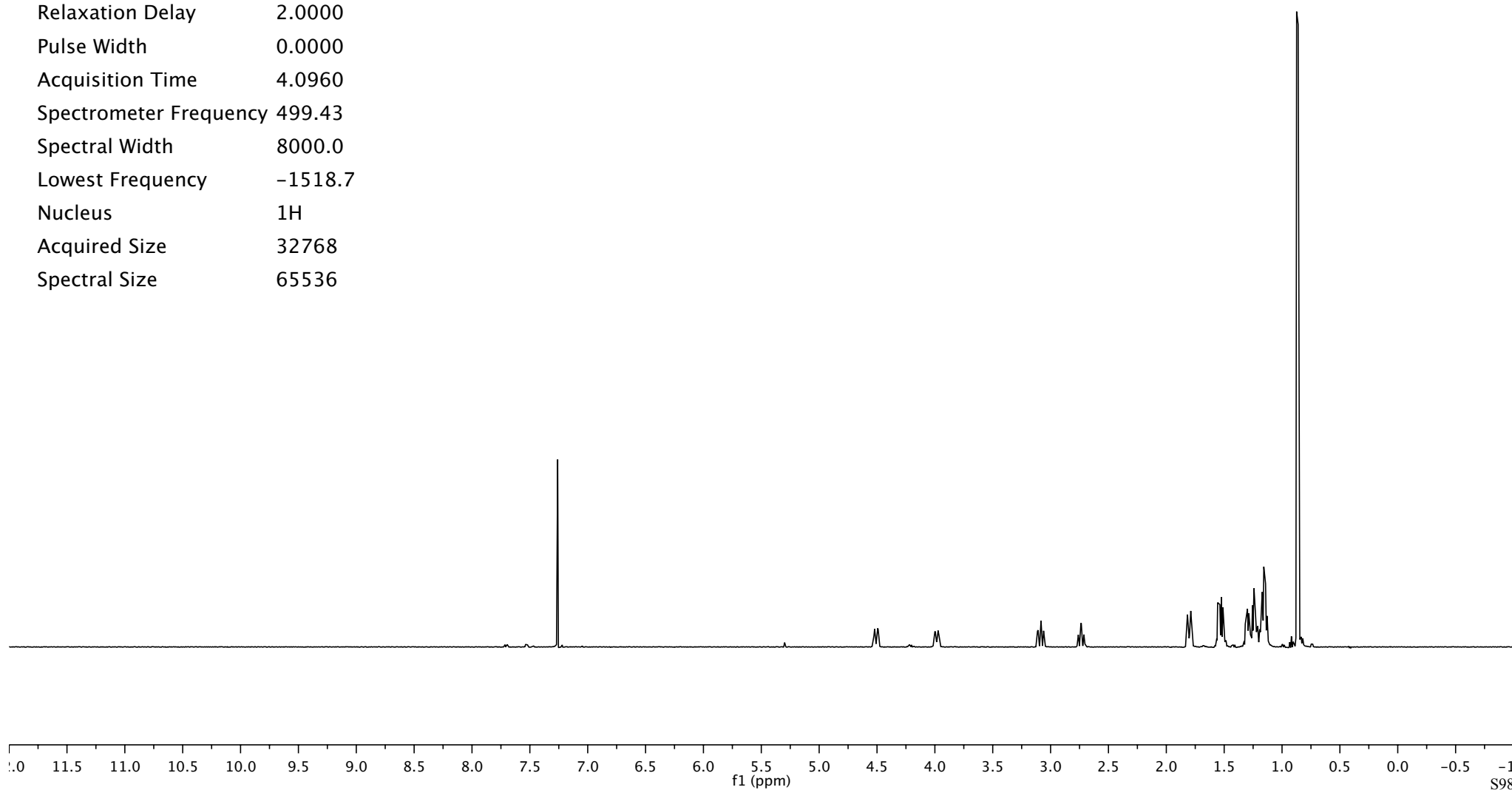
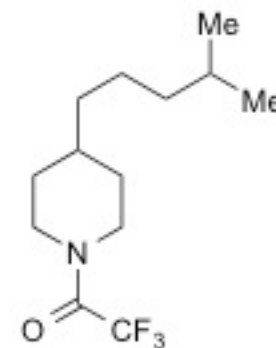
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24.49
22.76

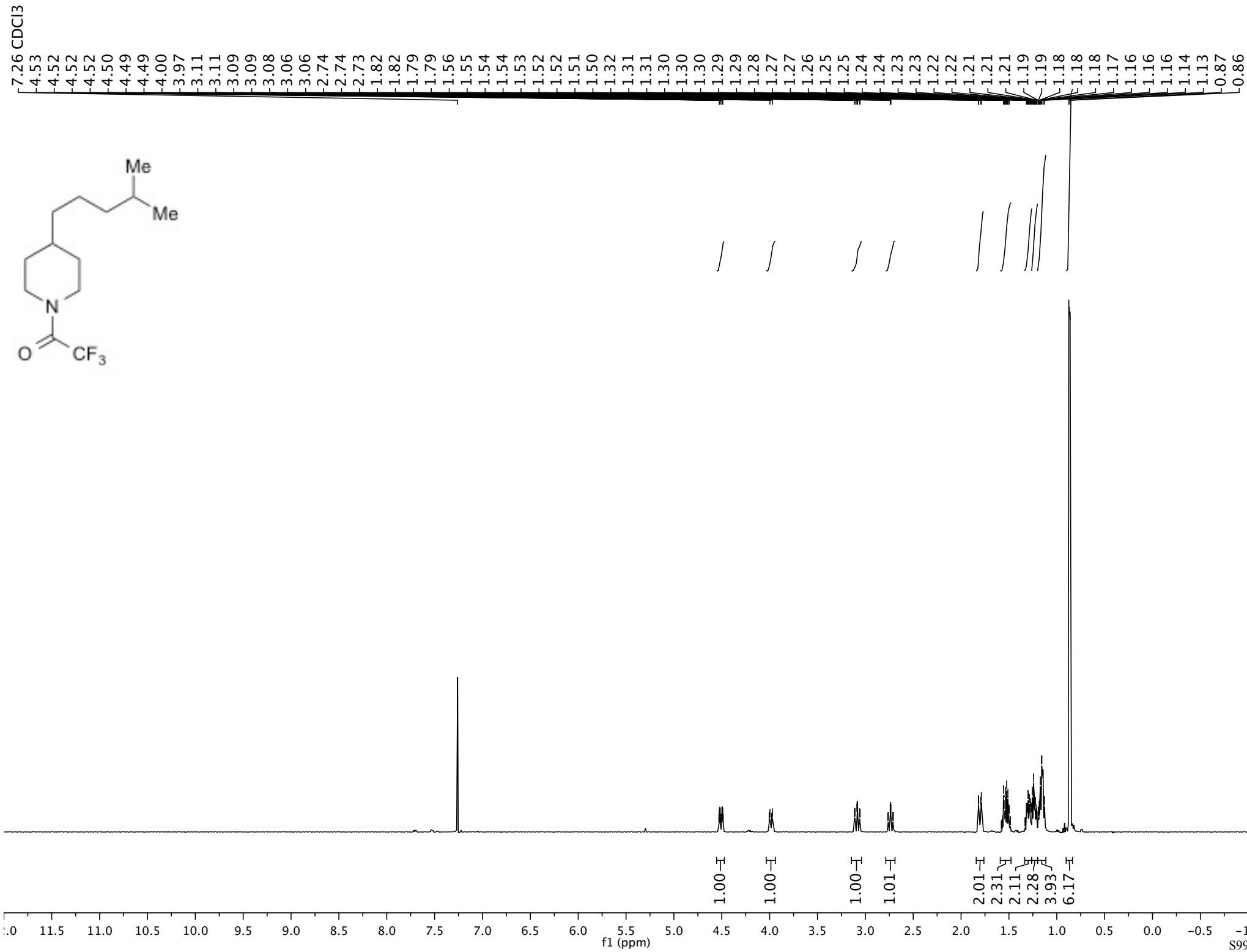
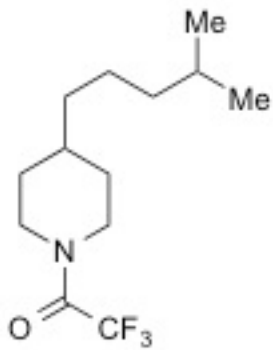
44.27



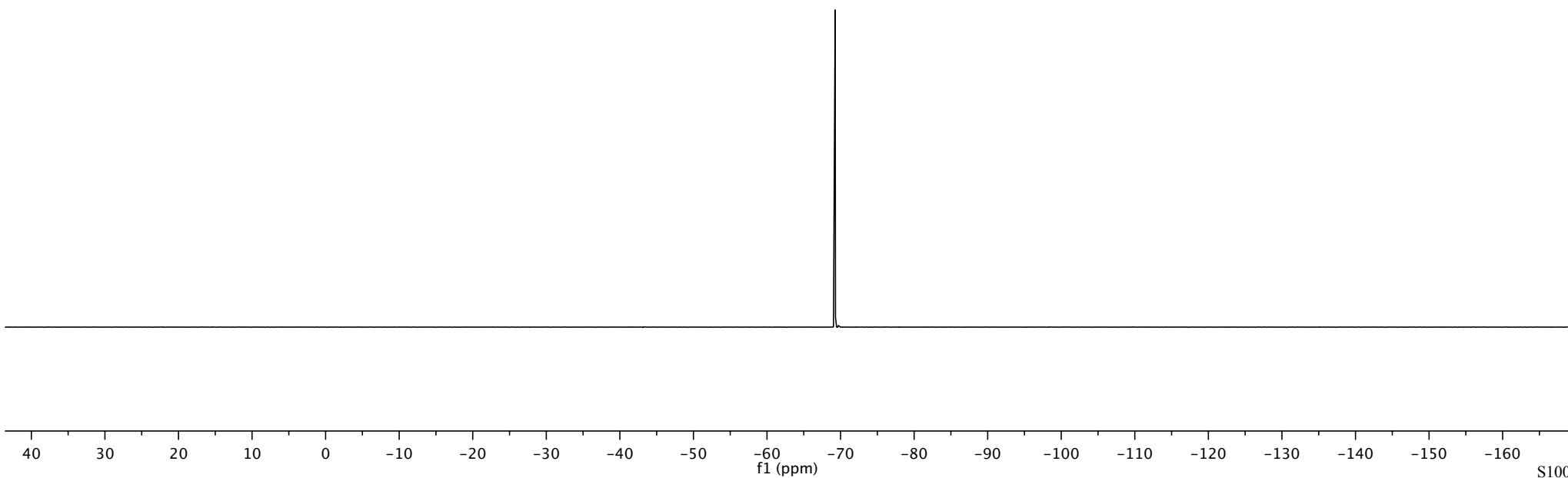
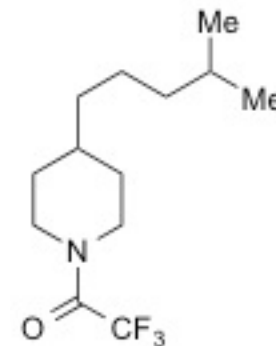
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f1 (ppm) S97

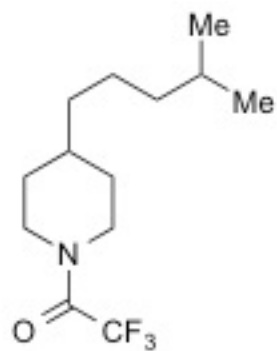
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Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Number of Scans	16
Receiver Gain	54
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	499.43
Spectral Width	8000.0
Lowest Frequency	-1518.7
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



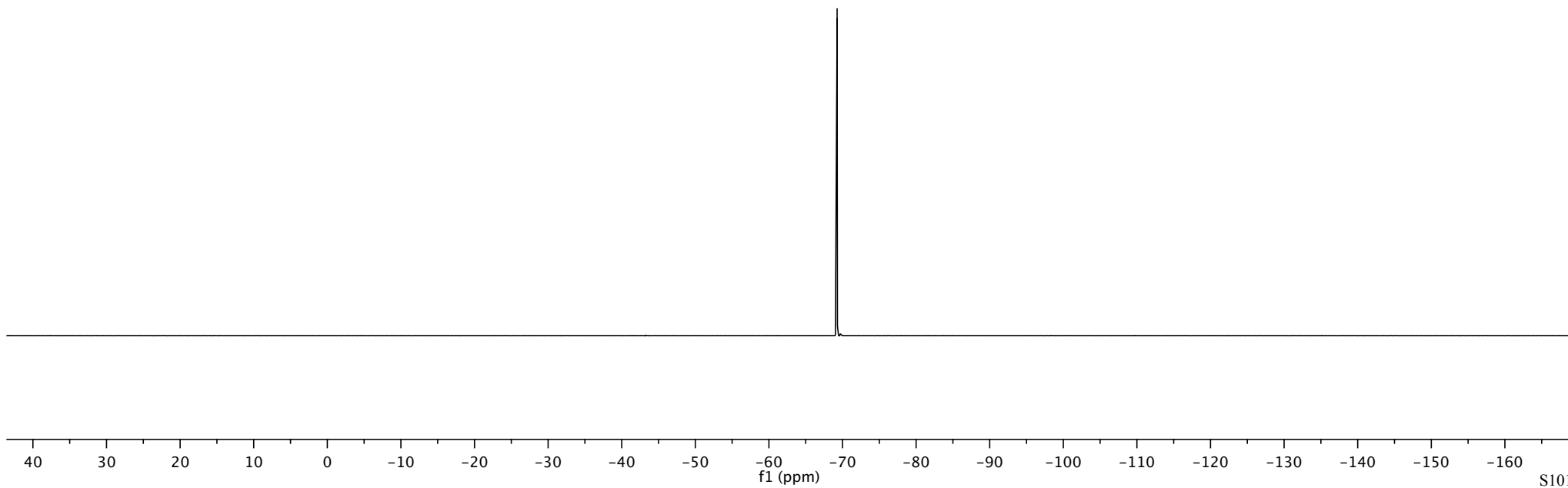


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	132
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency	-79501.3
Nucleus	¹⁹ F
Acquired Size	32768
Spectral Size	65536

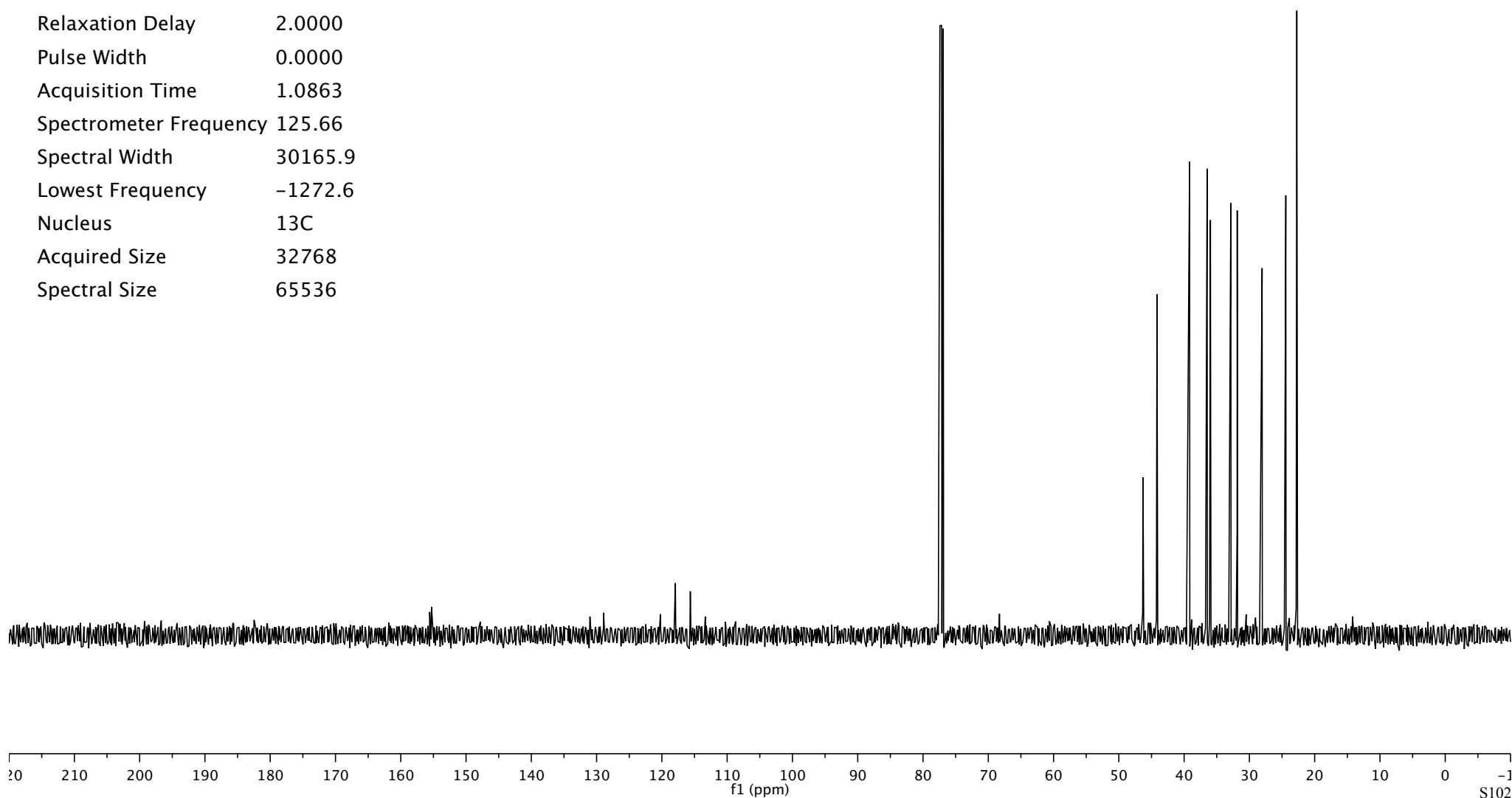
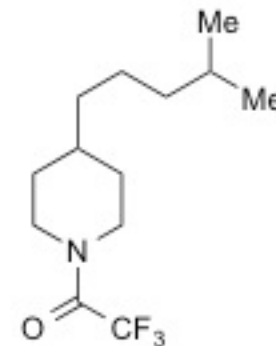


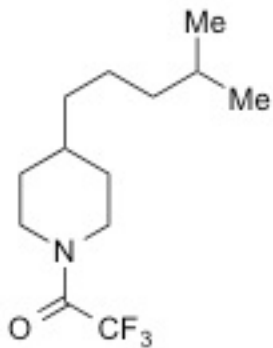


--69.27



Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	732
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1272.6
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



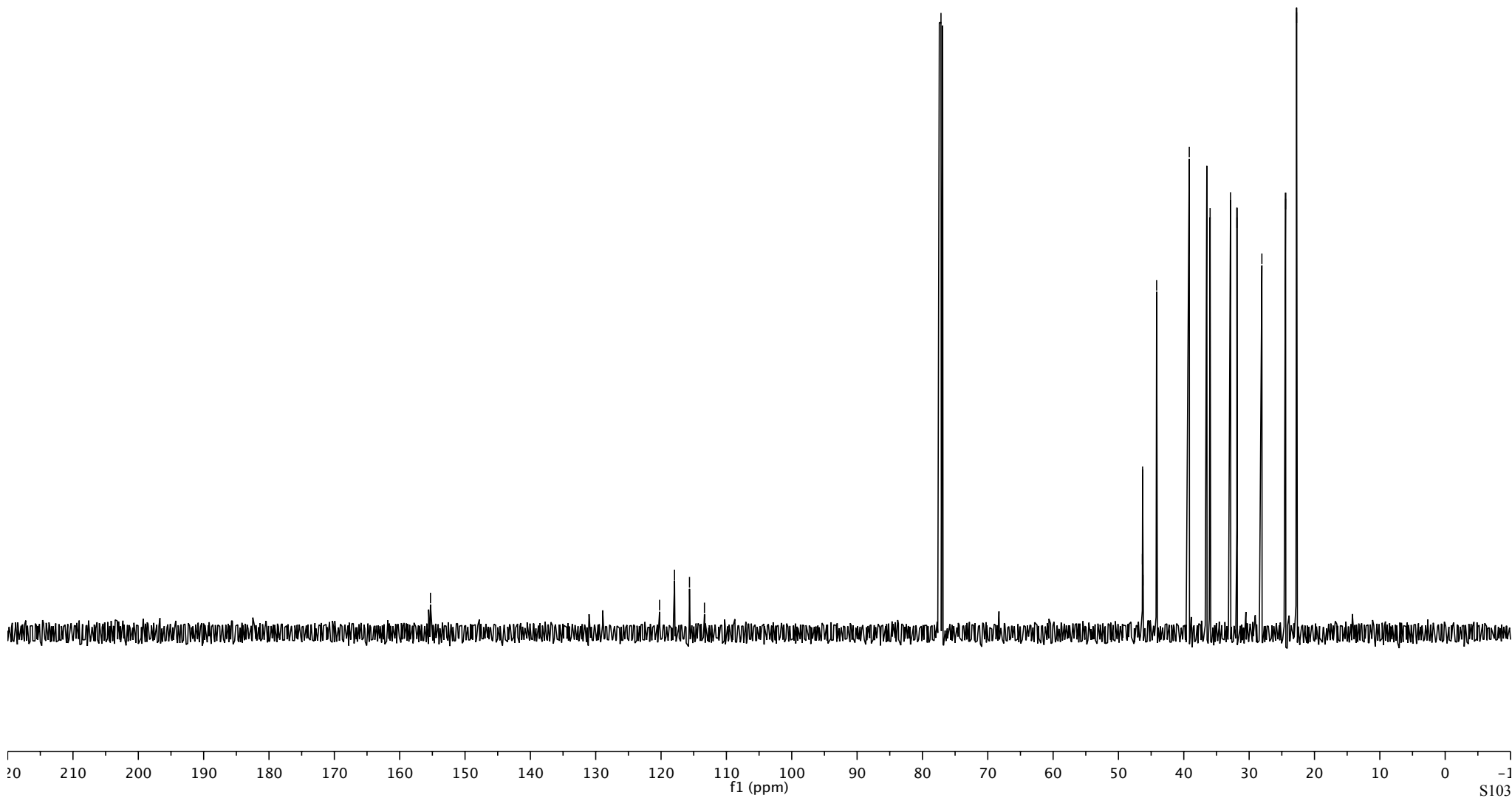


—155.29

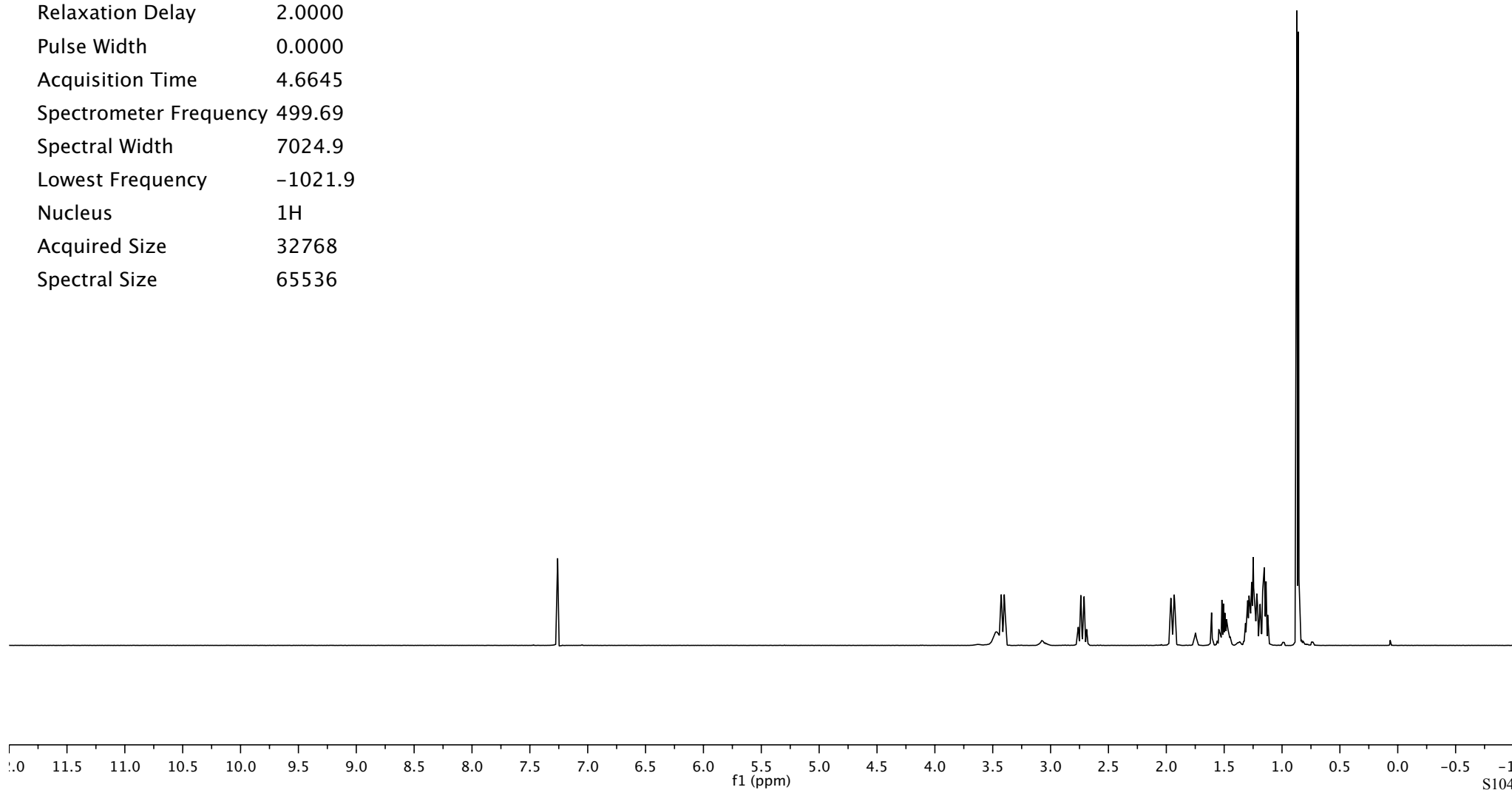
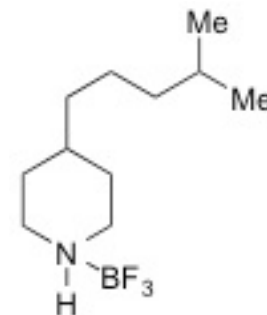
120.23
117.94
115.65
113.36

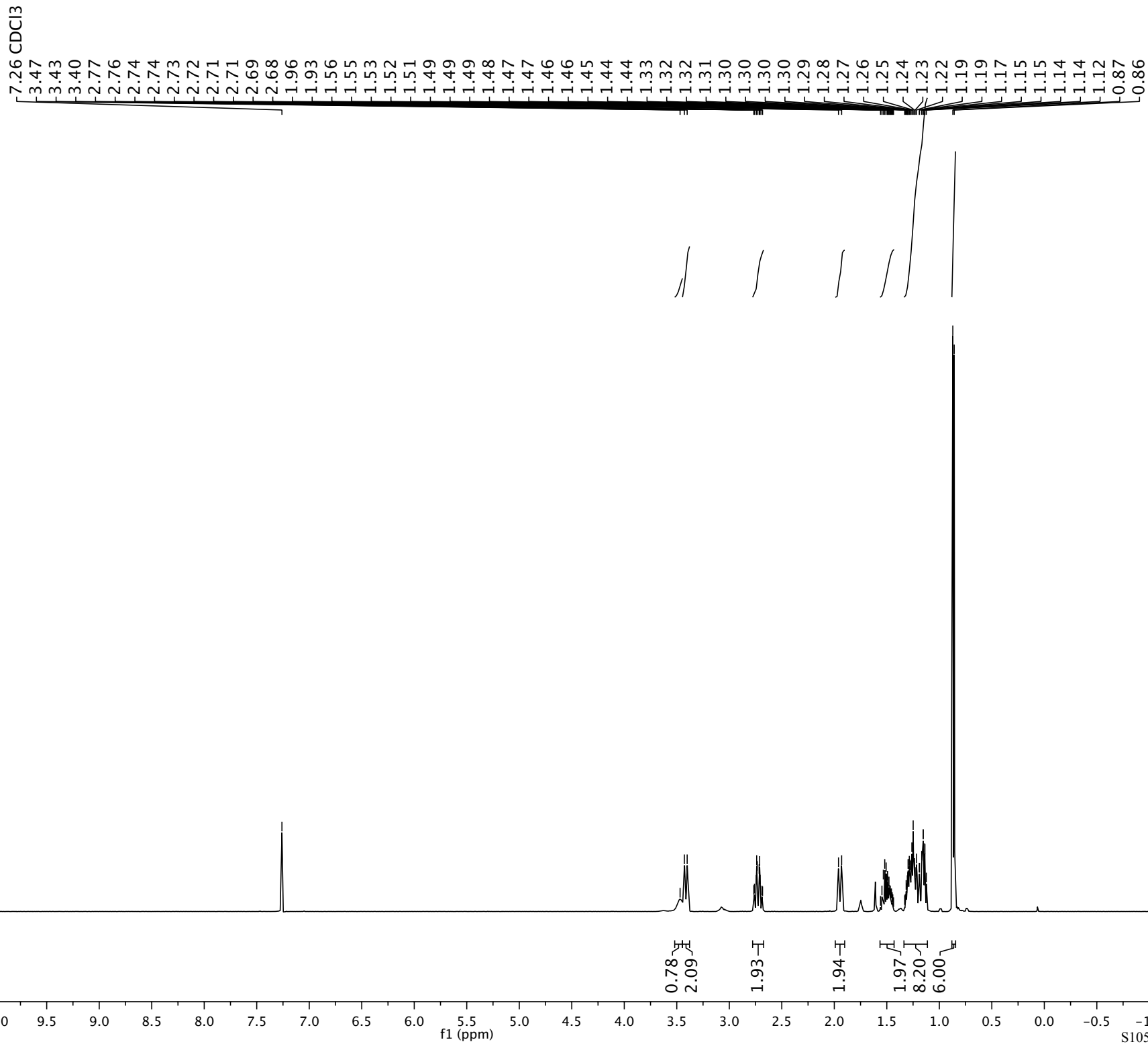
—77.16 CDCl₃

46.33
46.31
46.28
46.25
44.16
39.16
36.48
35.97
32.85
31.87
28.05
24.42
22.73

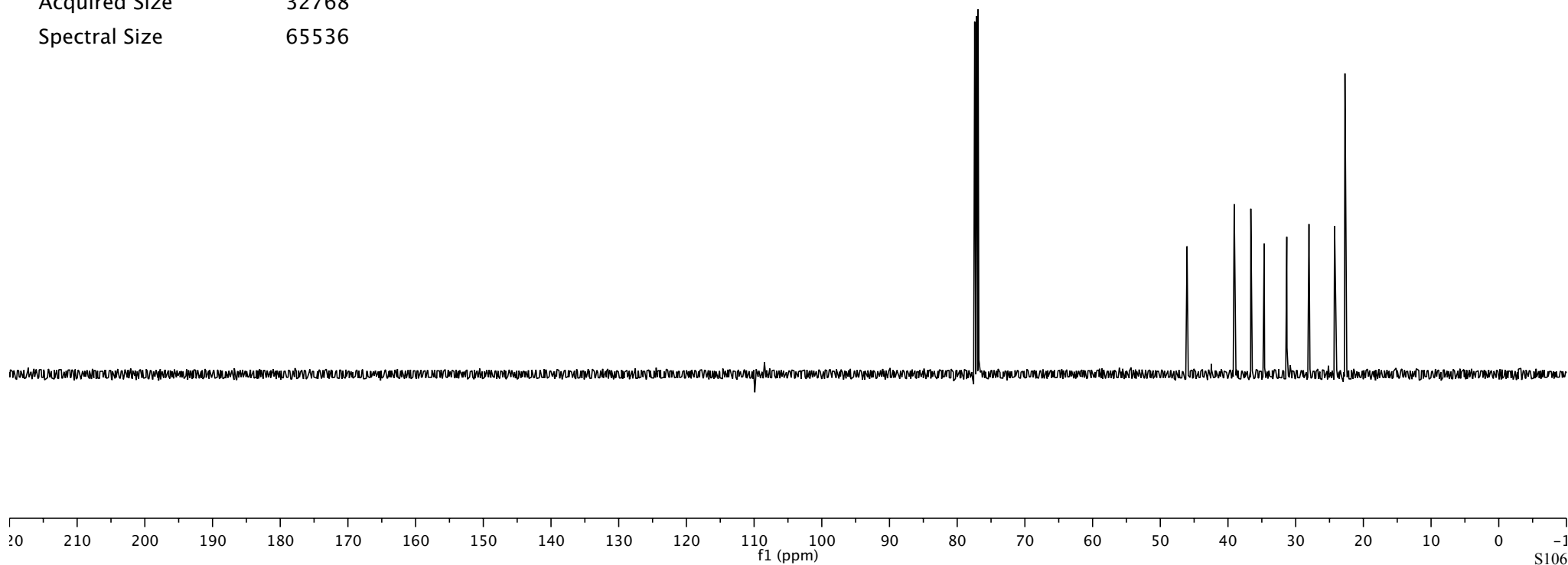
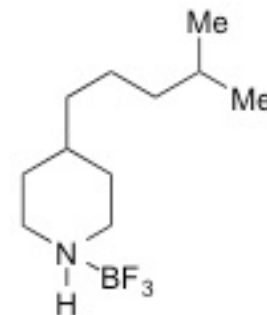


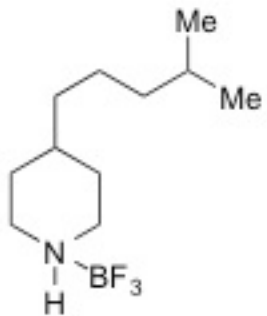
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	16
Receiver Gain	46
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.69
Spectral Width	7024.9
Lowest Frequency	-1021.9
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536





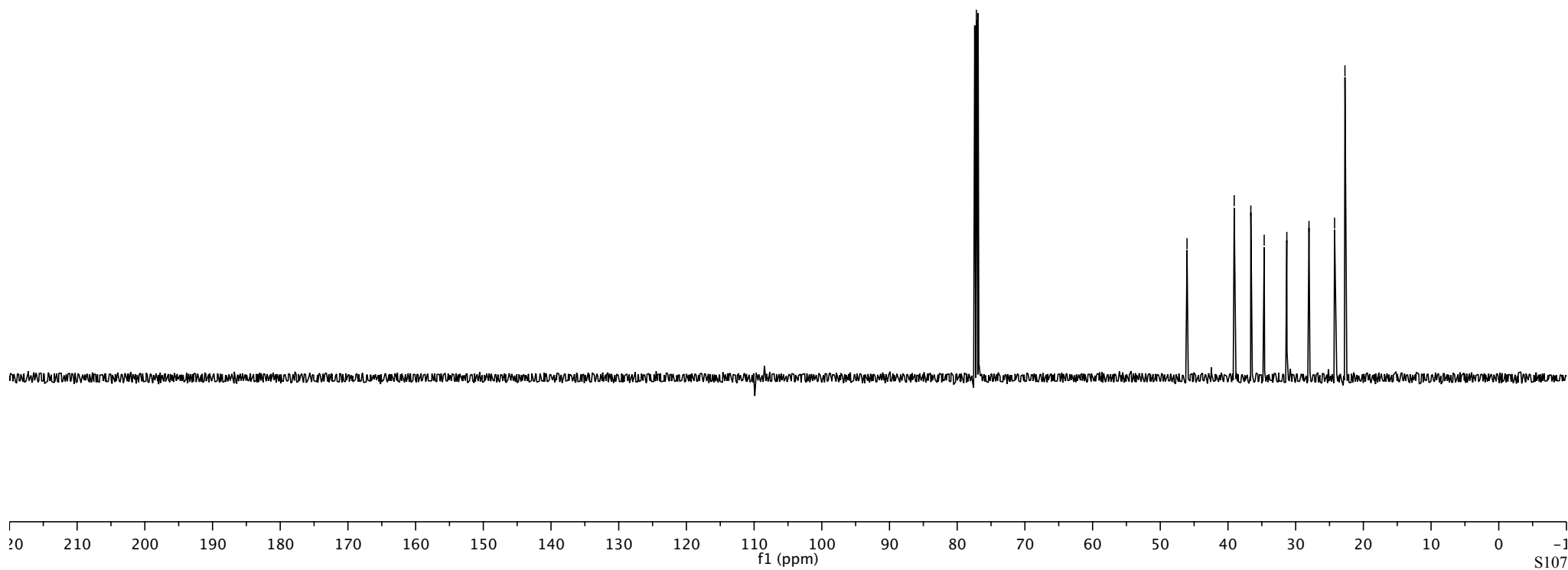
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Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	1012
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1272.5
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



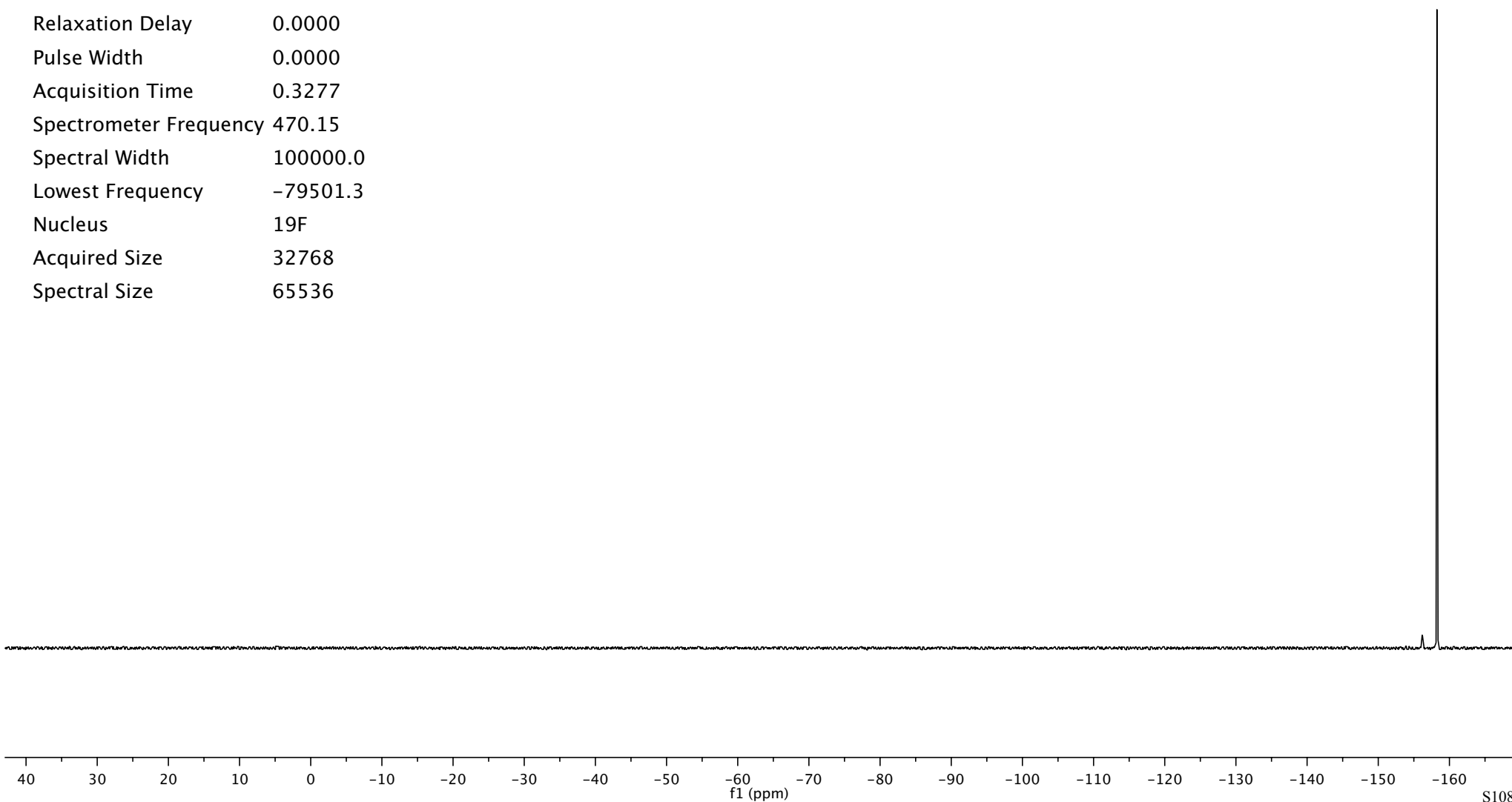
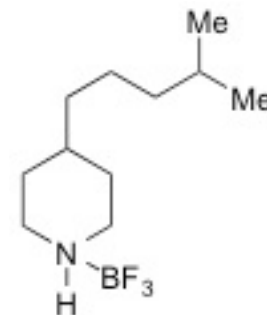


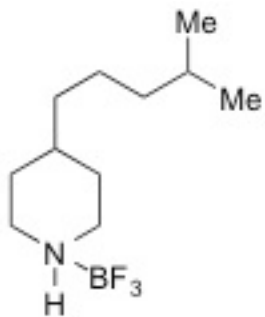
—77.16 CDCl₃

—46.05
—39.08
—36.62
—34.65
—31.31
—28.03
—24.25
—22.72



Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	132
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency	-79501.3
Nucleus	¹⁹ F
Acquired Size	32768
Spectral Size	65536



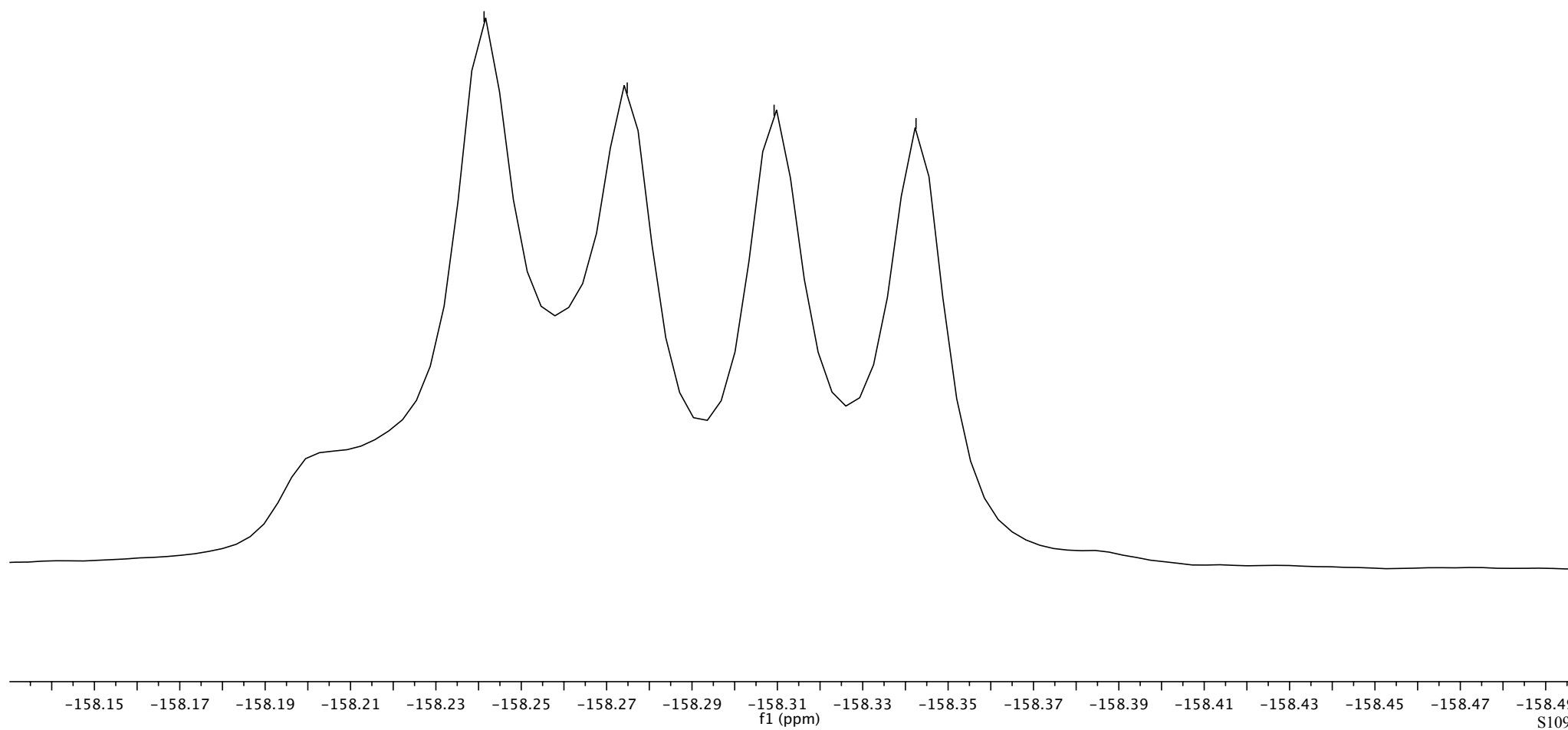


--158.24

--158.27

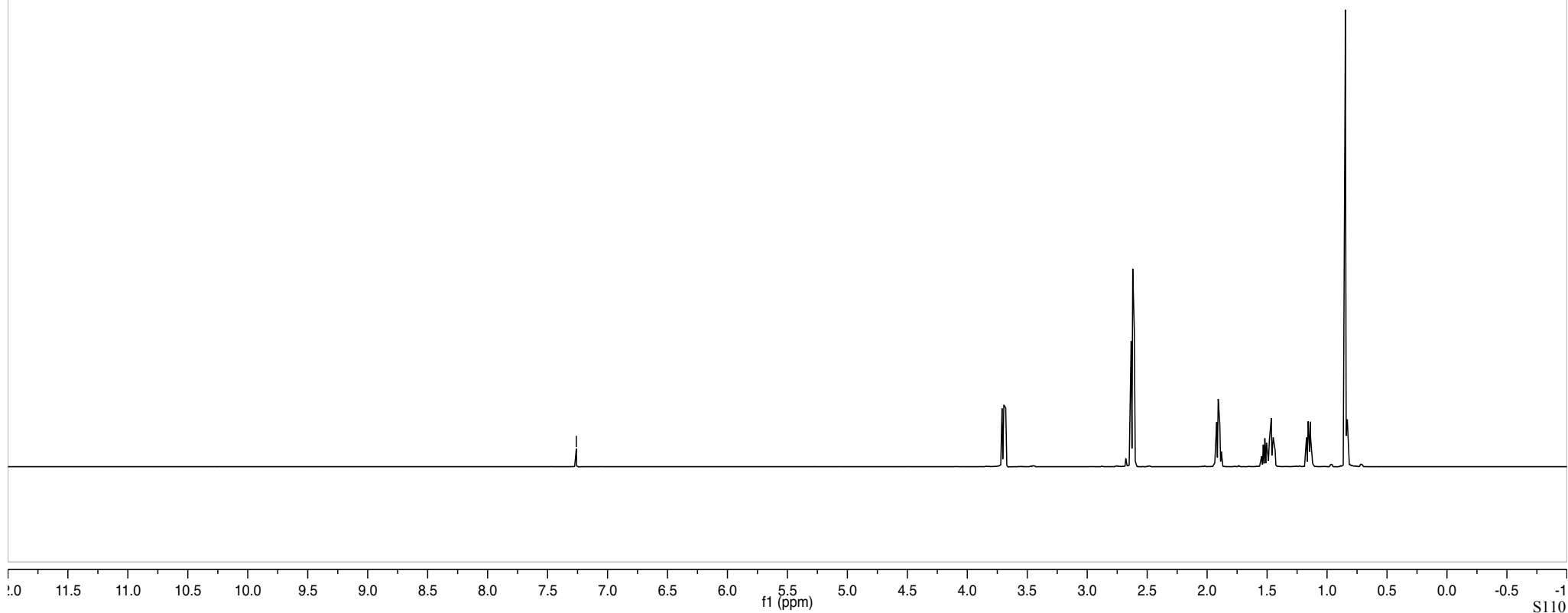
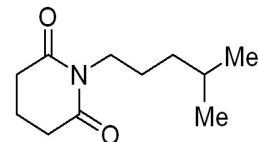
--158.31

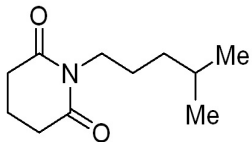
--158.34



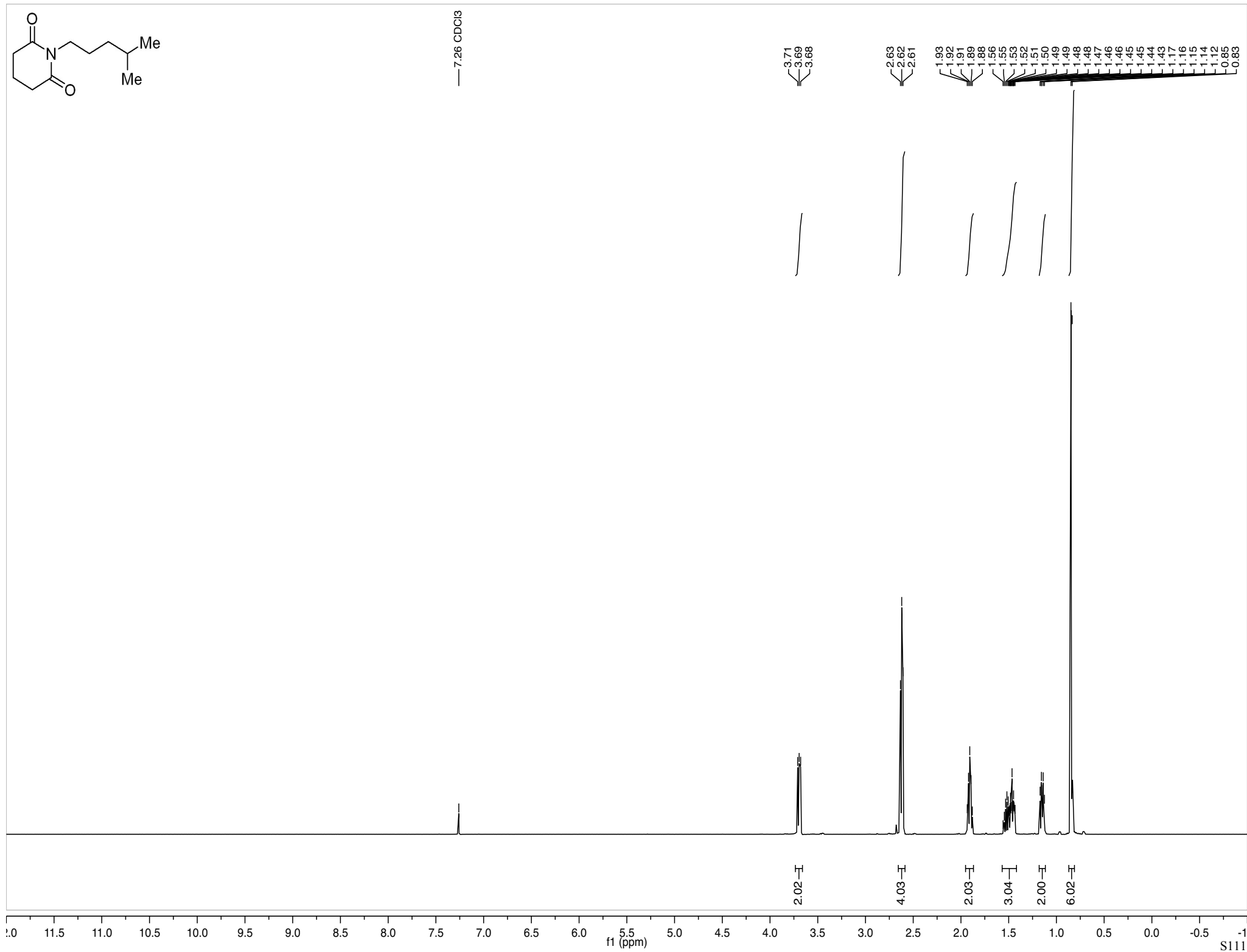
	Parameter	Value
1	Origin	Varian
2	Spectrometer	inova
3	Solvent	CDCl3
4	Temperature	20.0
5	Pulse Sequence	s2pul
6	Experiment	1D
7	Probe	QUAD
8	Number of Scans	8
9	Receiver Gain	41
10	Relaxation Delay	0.0000
11	Pulse Width	0.0000
12	Acquisition Time	4.6645
13	Spectrometer Frequency	499.69
14	Spectral Width	7024.9
15	Lowest Frequency	-1011.4
16	Nucleus	¹ H
17	Acquired Size	32768
18	Spectral Size	65536

— 7.26 CDCl₃



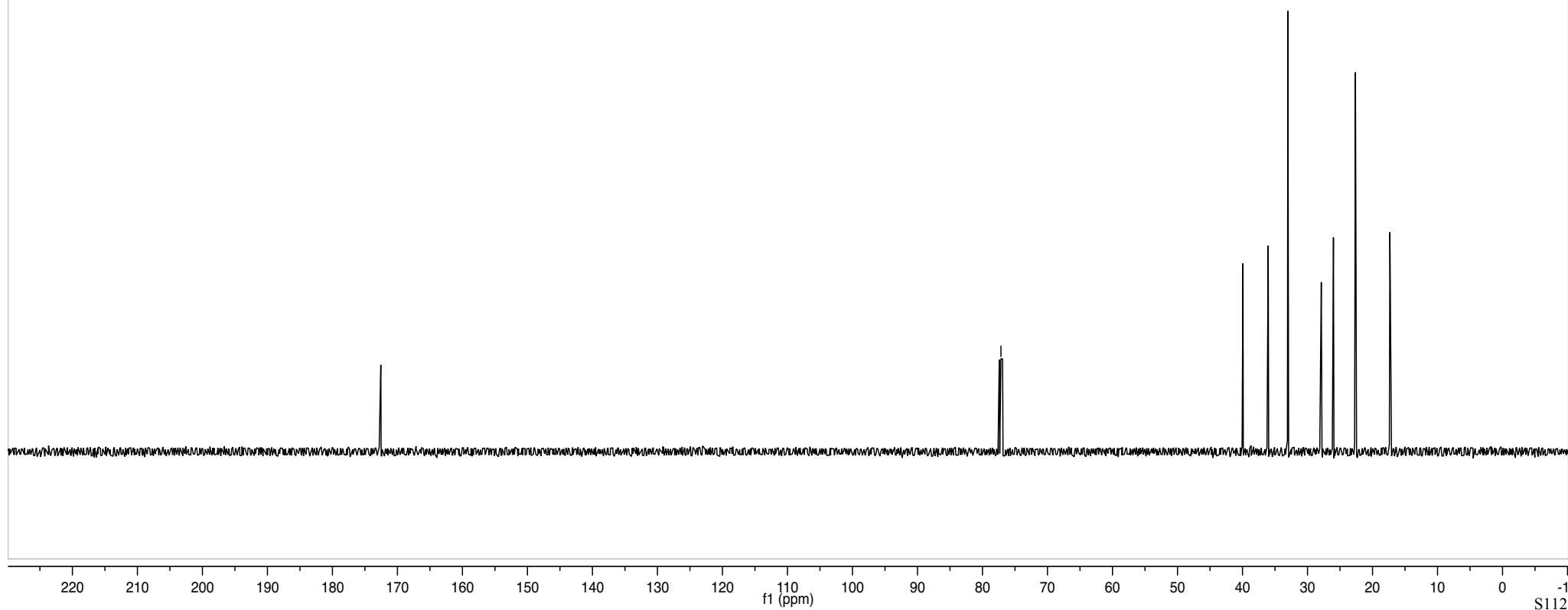
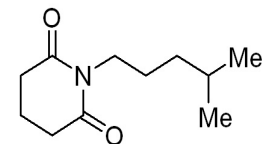


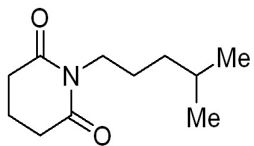
— 7.26 CDCl₃



Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	80
9 Receiver Gain	60
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.0863
13 Spectrometer Frequency	125.66
14 Spectral Width	30165.9
15 Lowest Frequency	-1274.3
16 Nucleus	13C
17 Acquired Size	32768
18 Spectral Size	65536

— 77.2 CDCl3

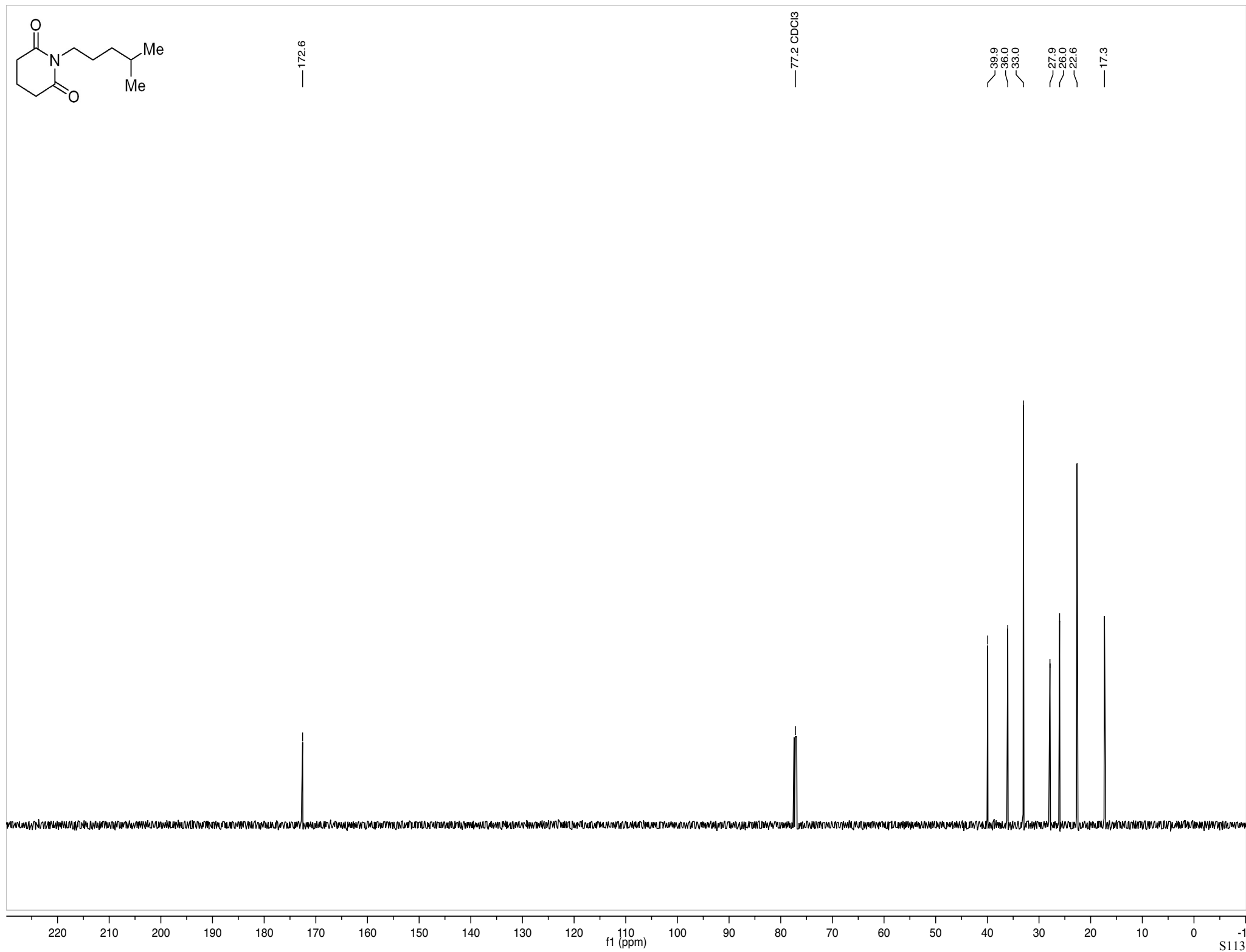


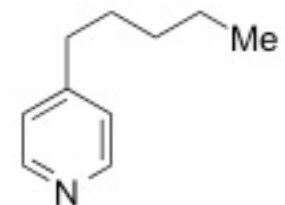


—172.6

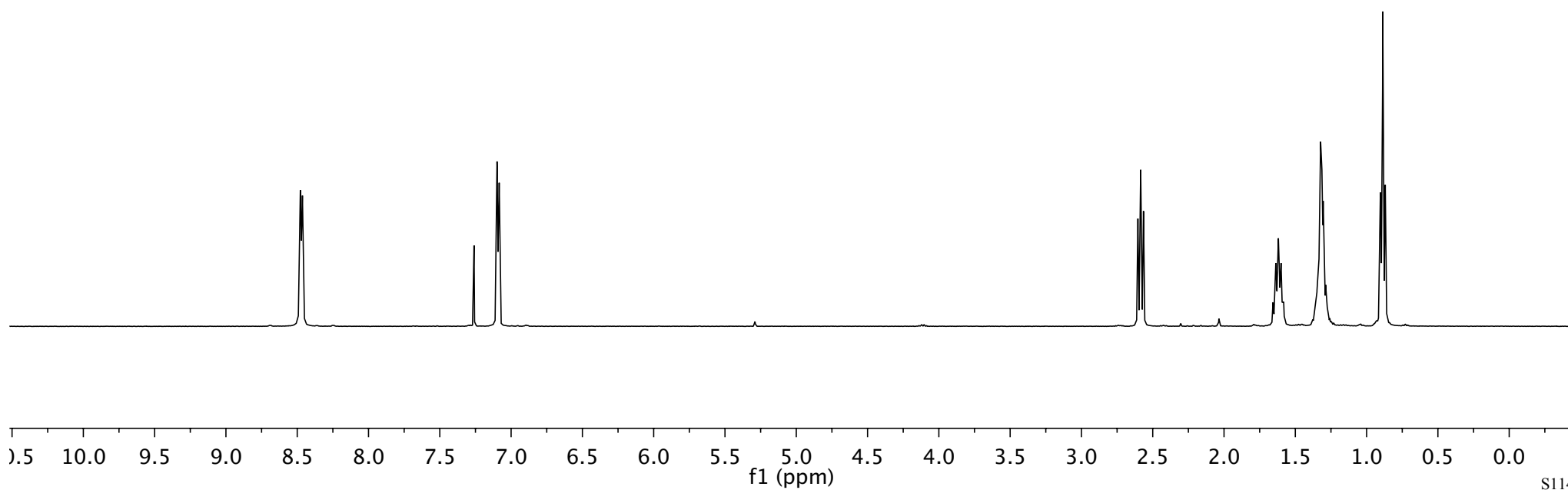
—77.2 CDCl₃

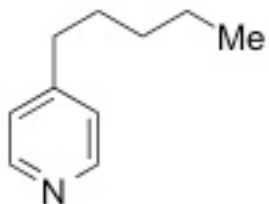
39.9
36.0
33.0
27.9
26.0
22.6
—17.3





Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	5mmsw
Receiver Gain	52
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	399.74
Spectral Width	8000.0
Lowest Frequency	-2421.6
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536





8.48
8.46

7.26 CDCl₃
7.10
7.08

2.60
2.58
2.56
1.66
1.64
1.62
1.60
1.58
1.37
1.36
1.34
1.33
1.32
1.31
1.30
1.30
1.29
1.28
1.27
0.90
0.89
0.87

1.92

1.87

2.00

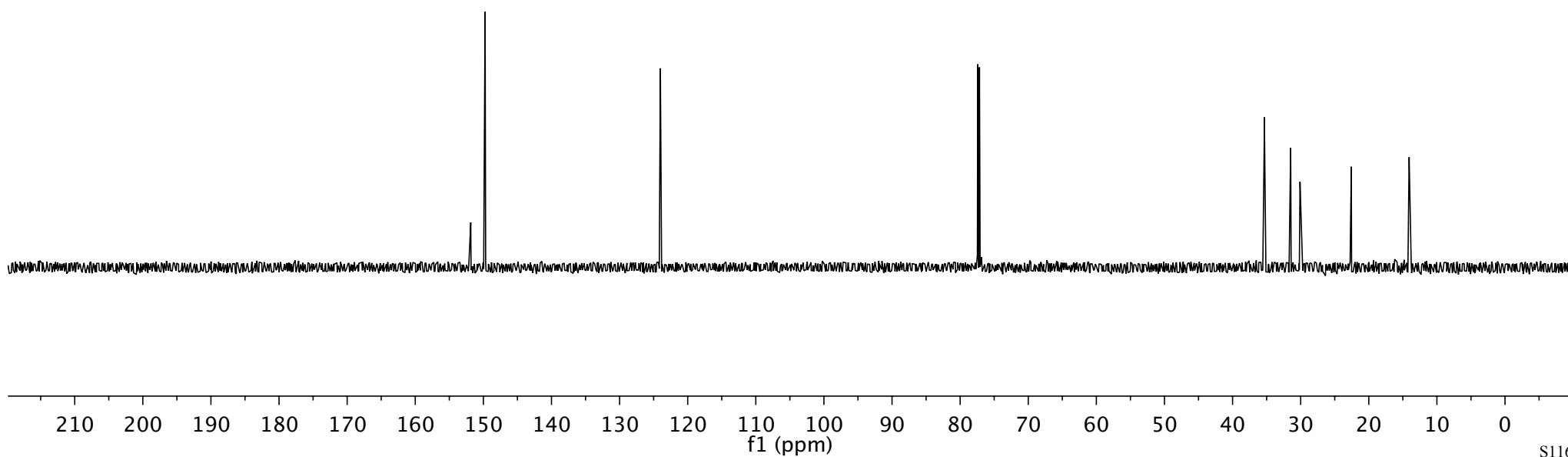
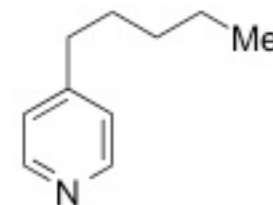
2.02

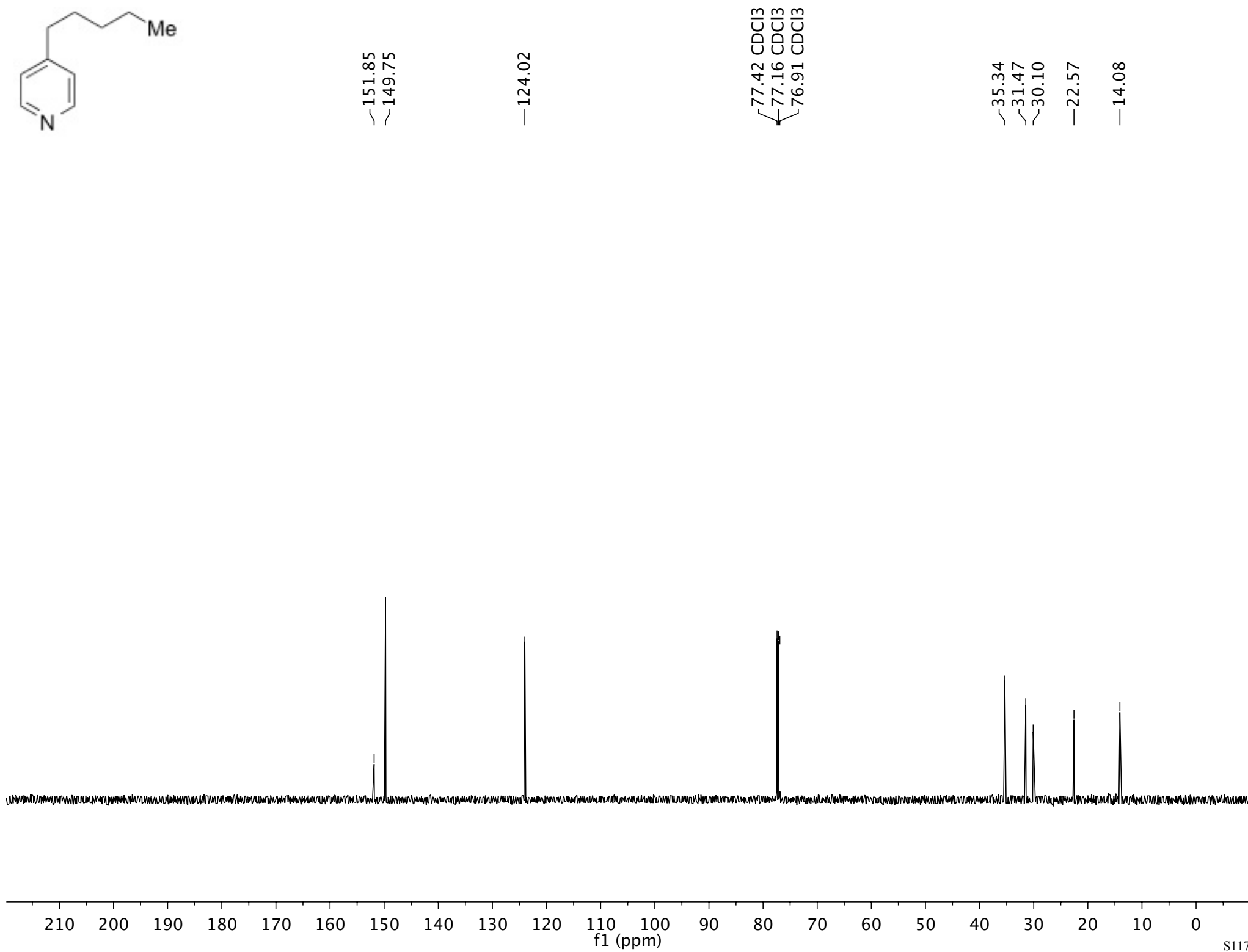
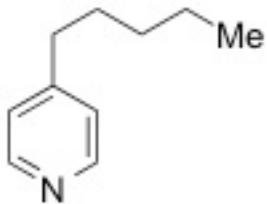
4.13

3.08

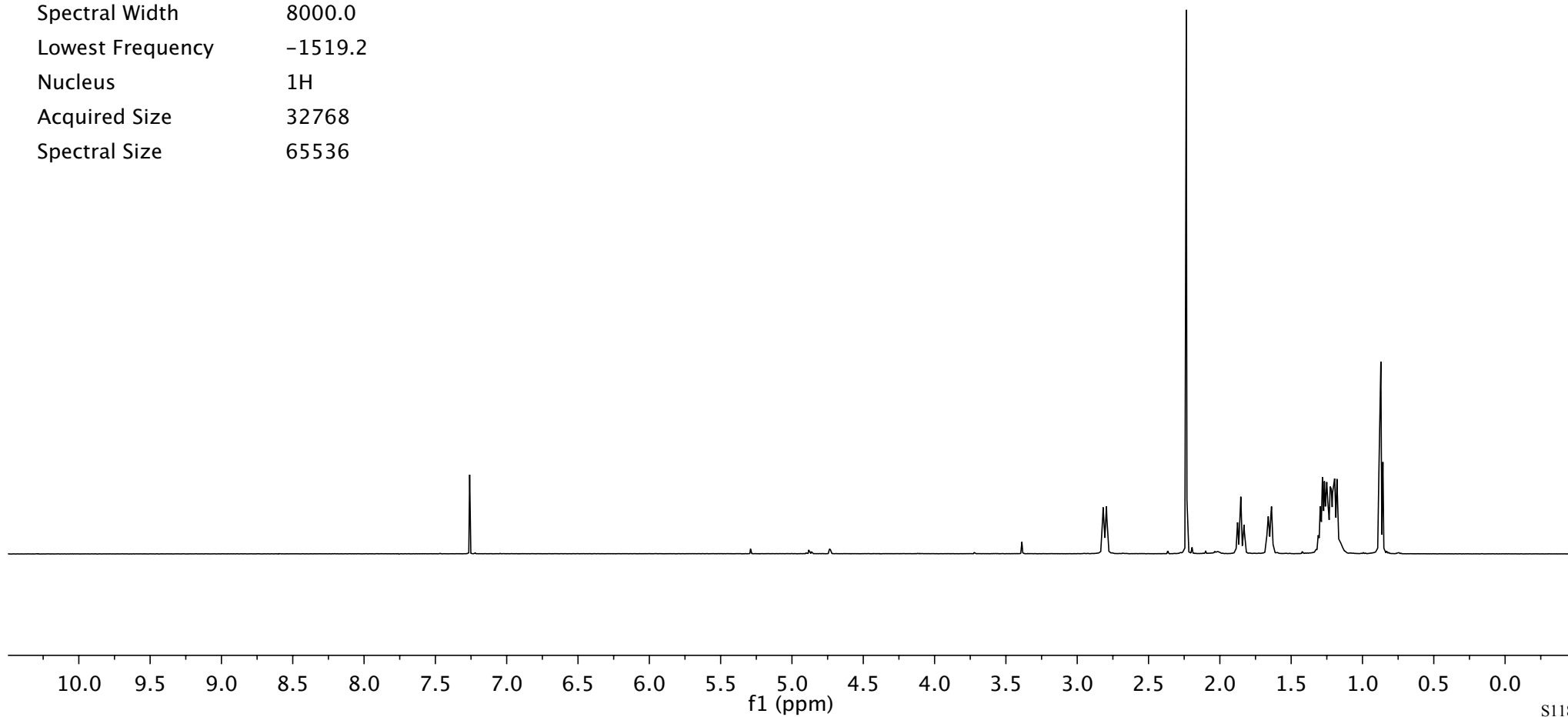
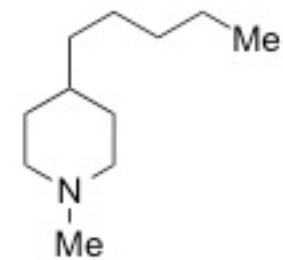
f1 (ppm)

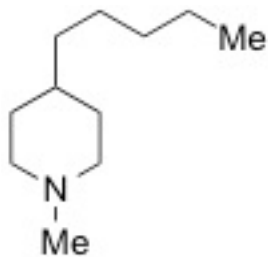
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2200.5
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



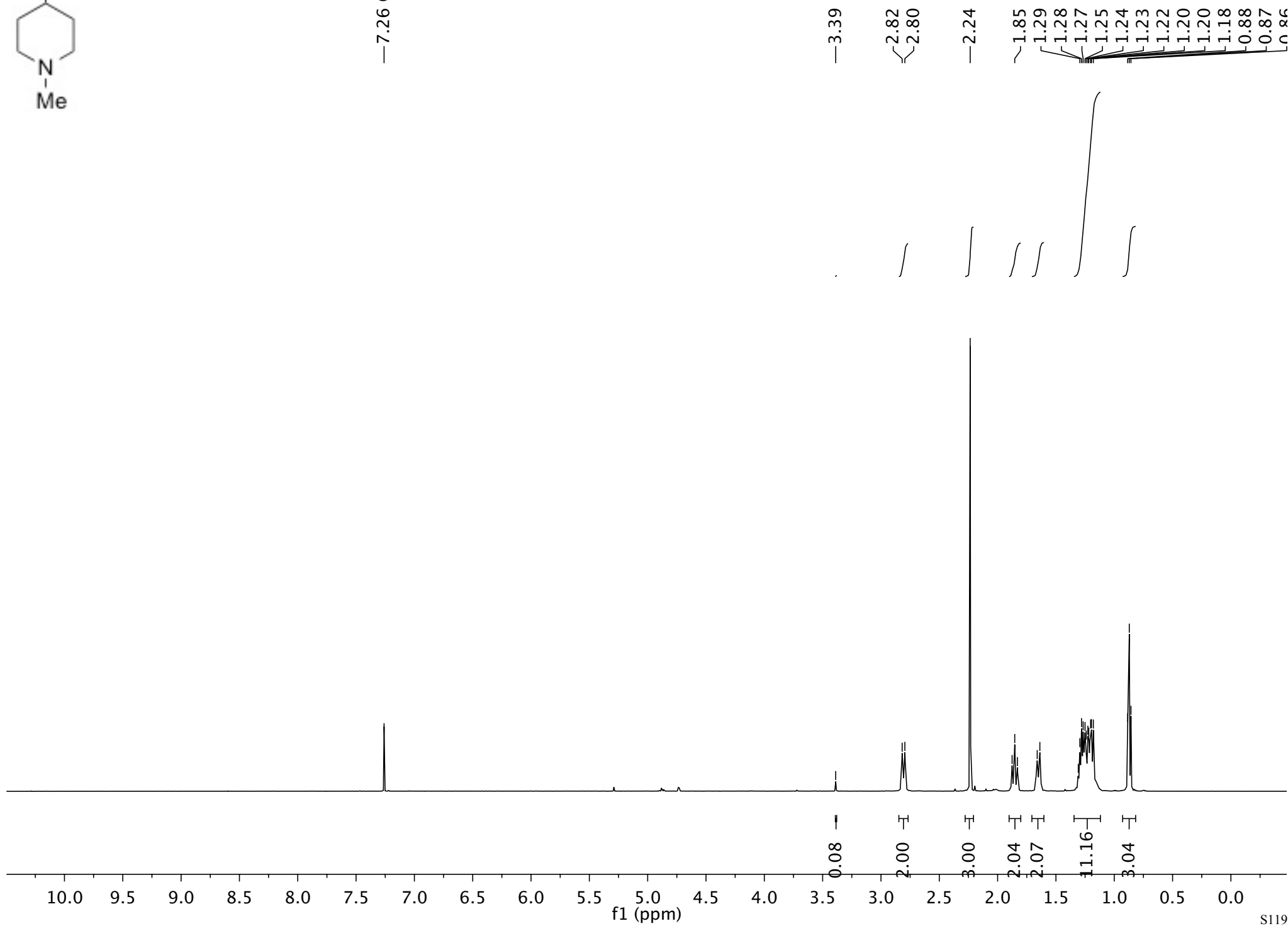


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	50
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	499.43
Spectral Width	8000.0
Lowest Frequency	-1519.2
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

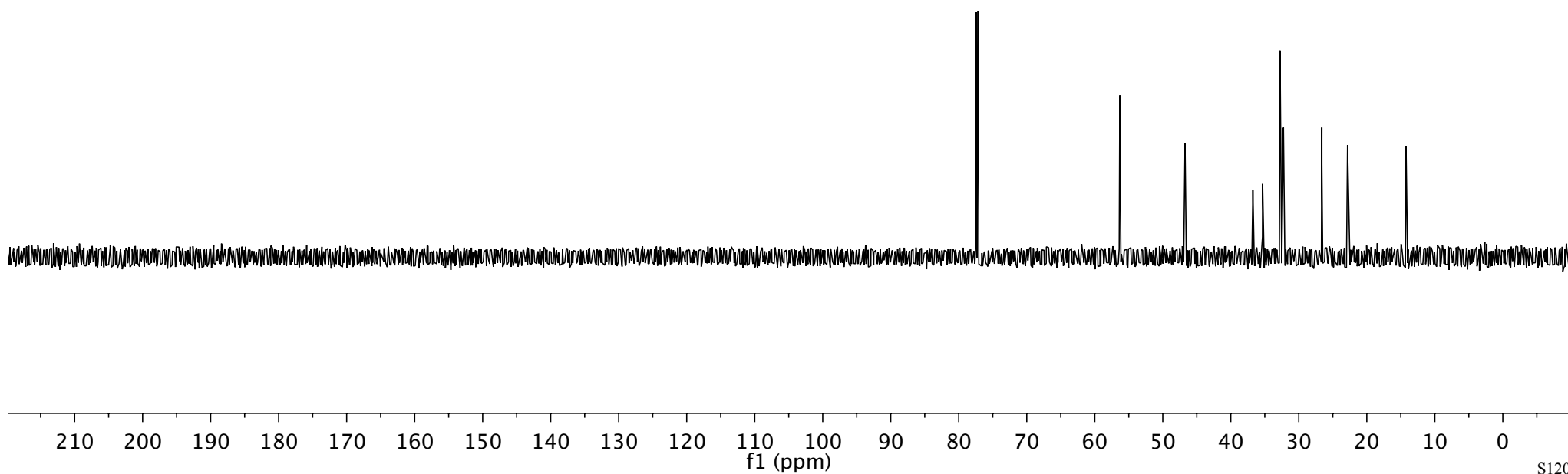
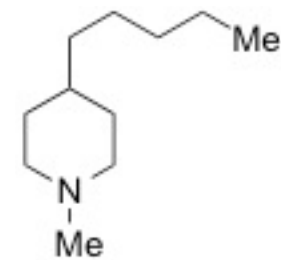


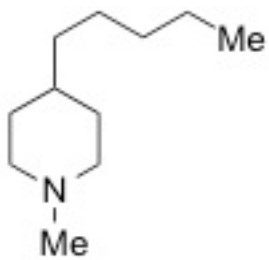


—7.26 CDCl₃



Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2200.1
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536





77.41 CDCl₃
77.16 CDCl₃
76.91 CDCl₃

—56.32

—46.73

36.75

—35.32

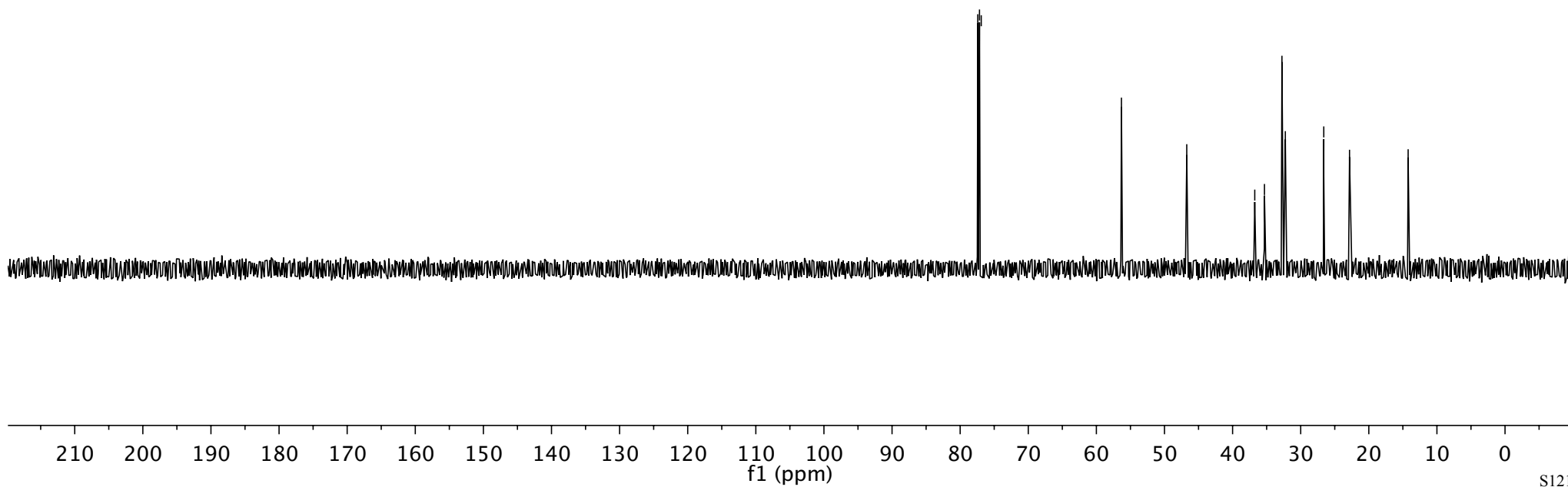
32.75

32.26

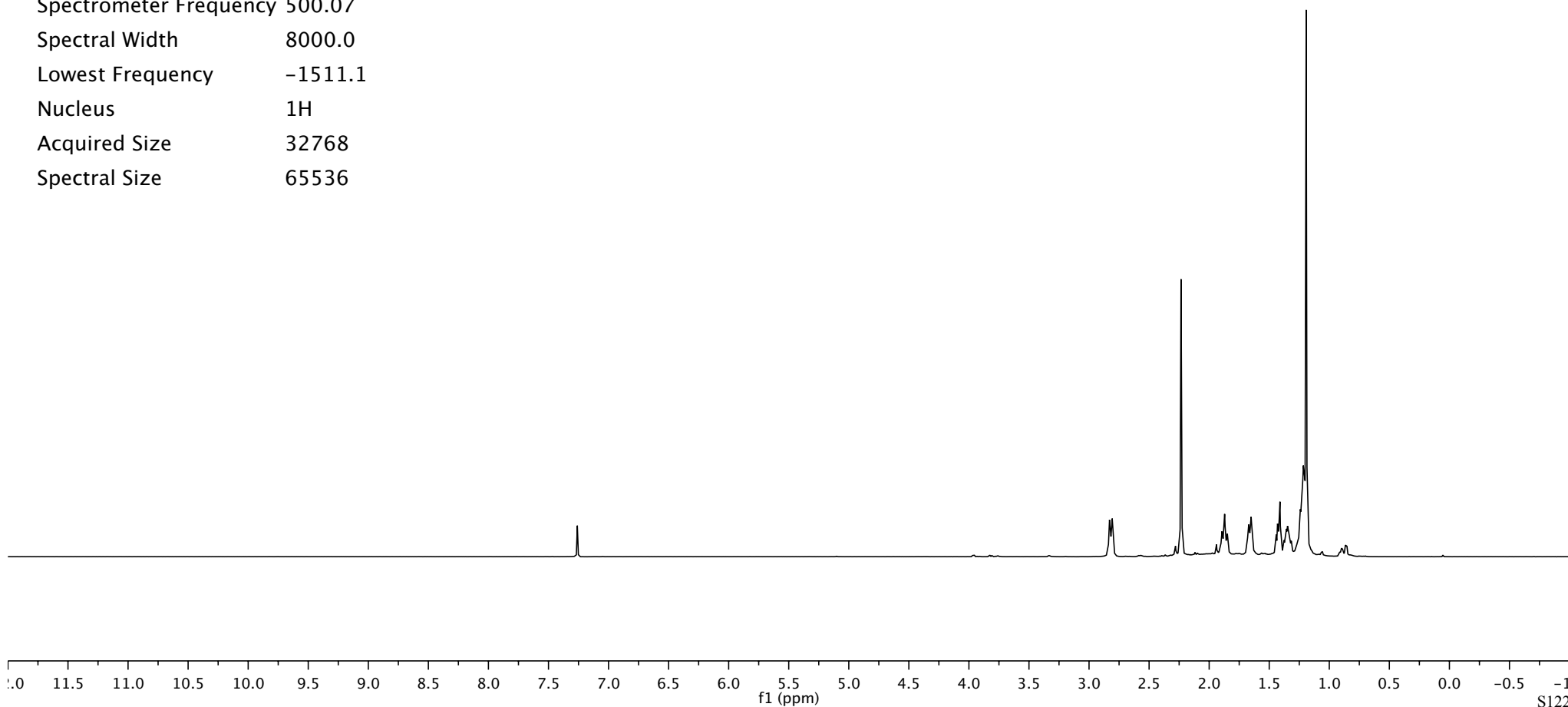
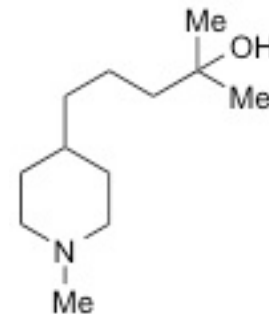
26.61

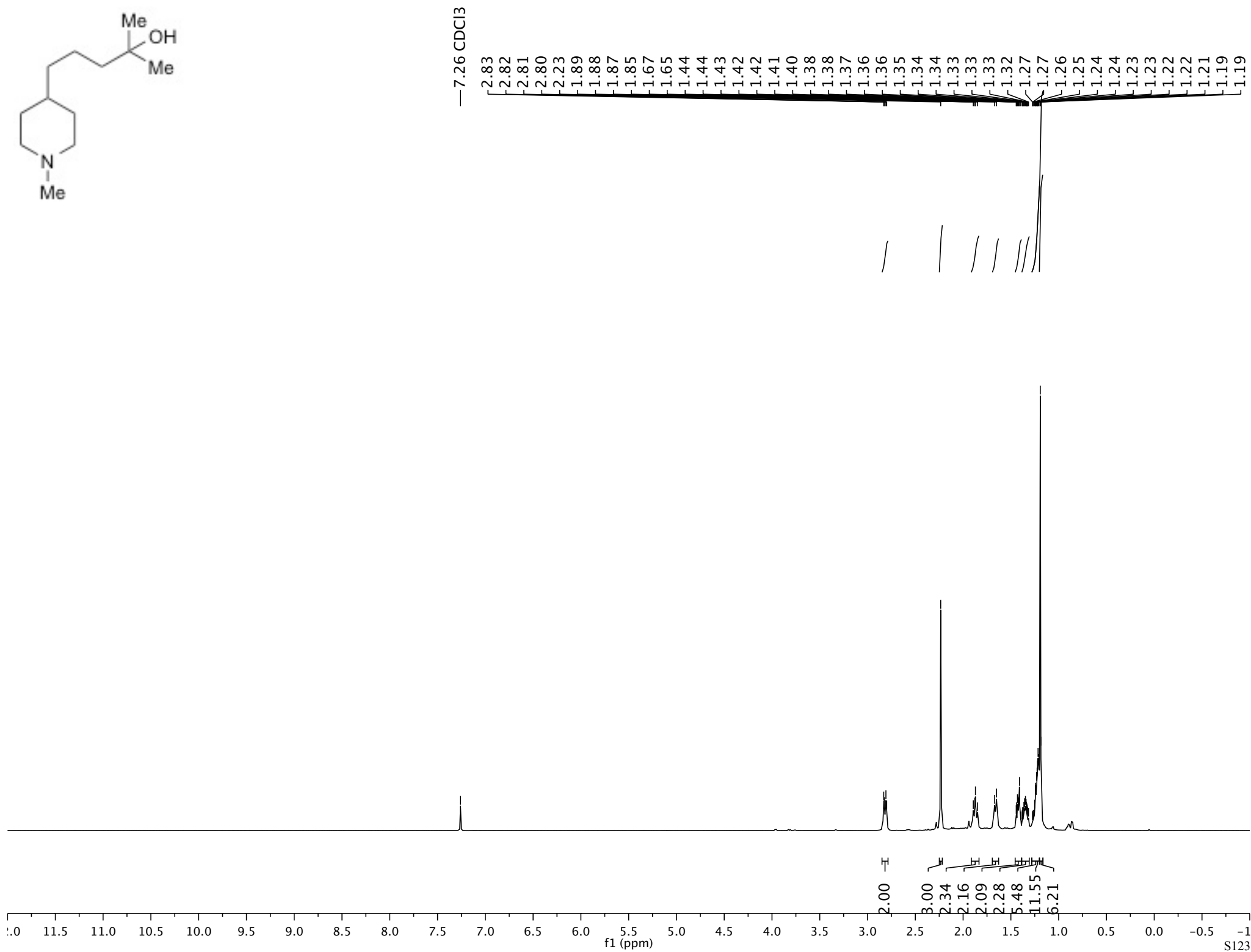
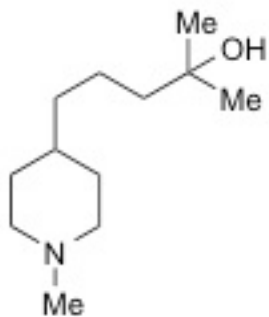
22.83

—14.22

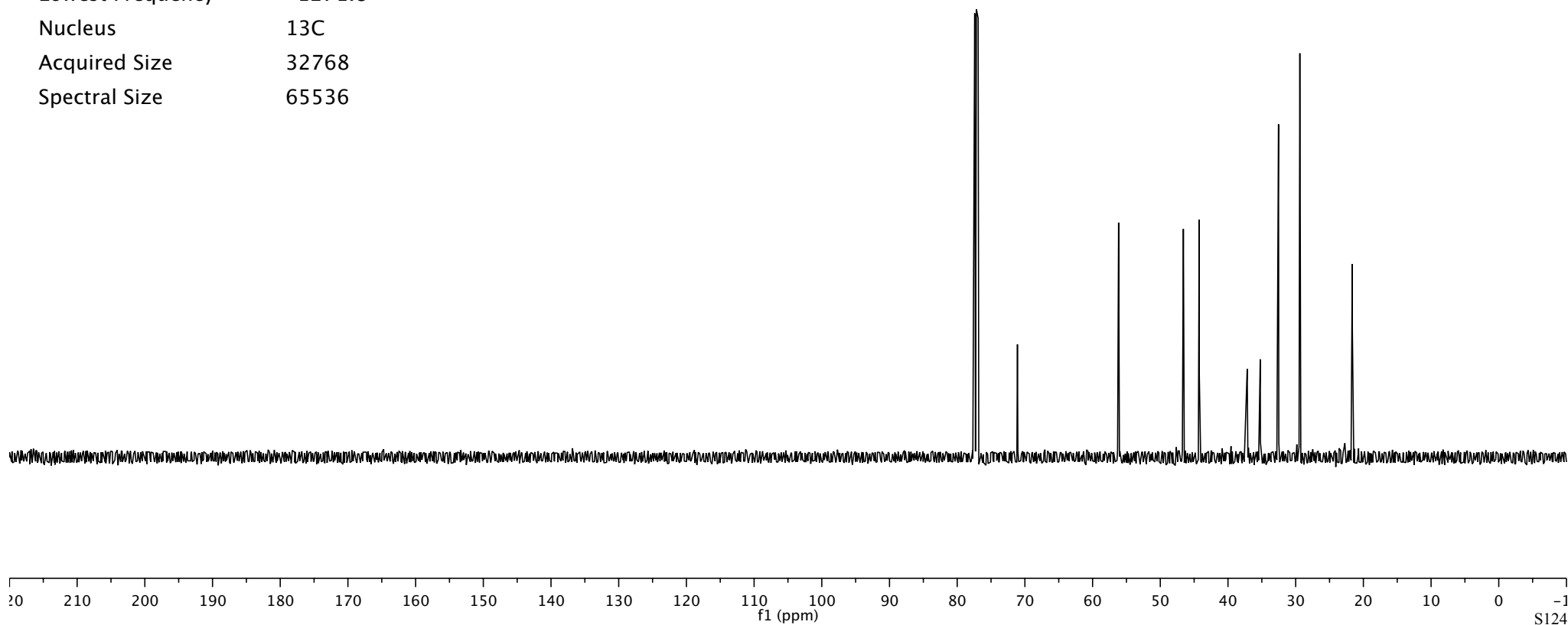
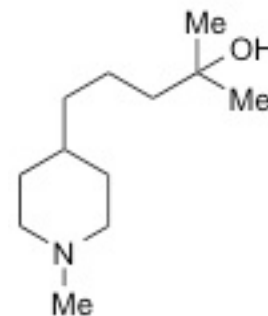


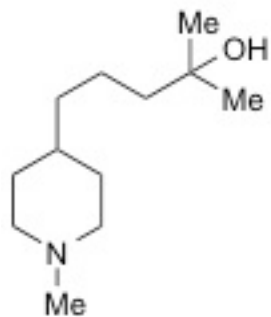
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	26
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1511.1
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



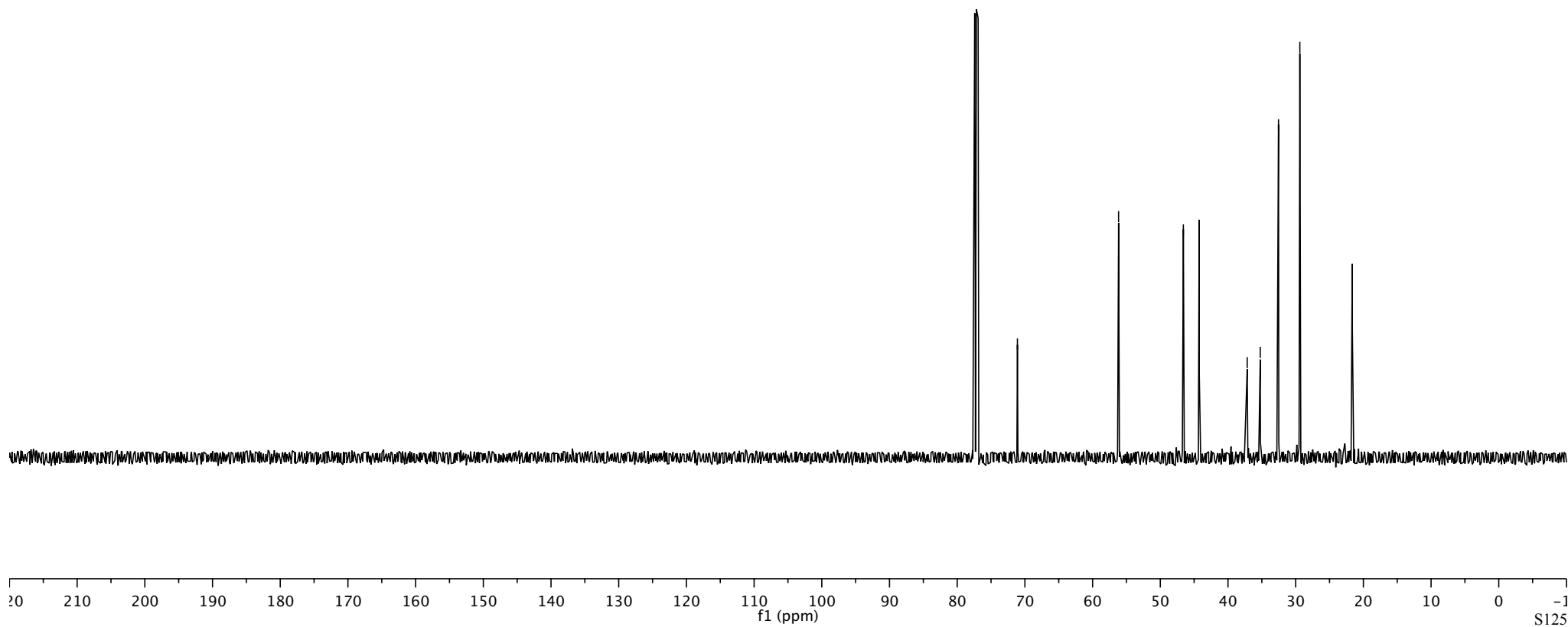


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	512
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1271.8
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

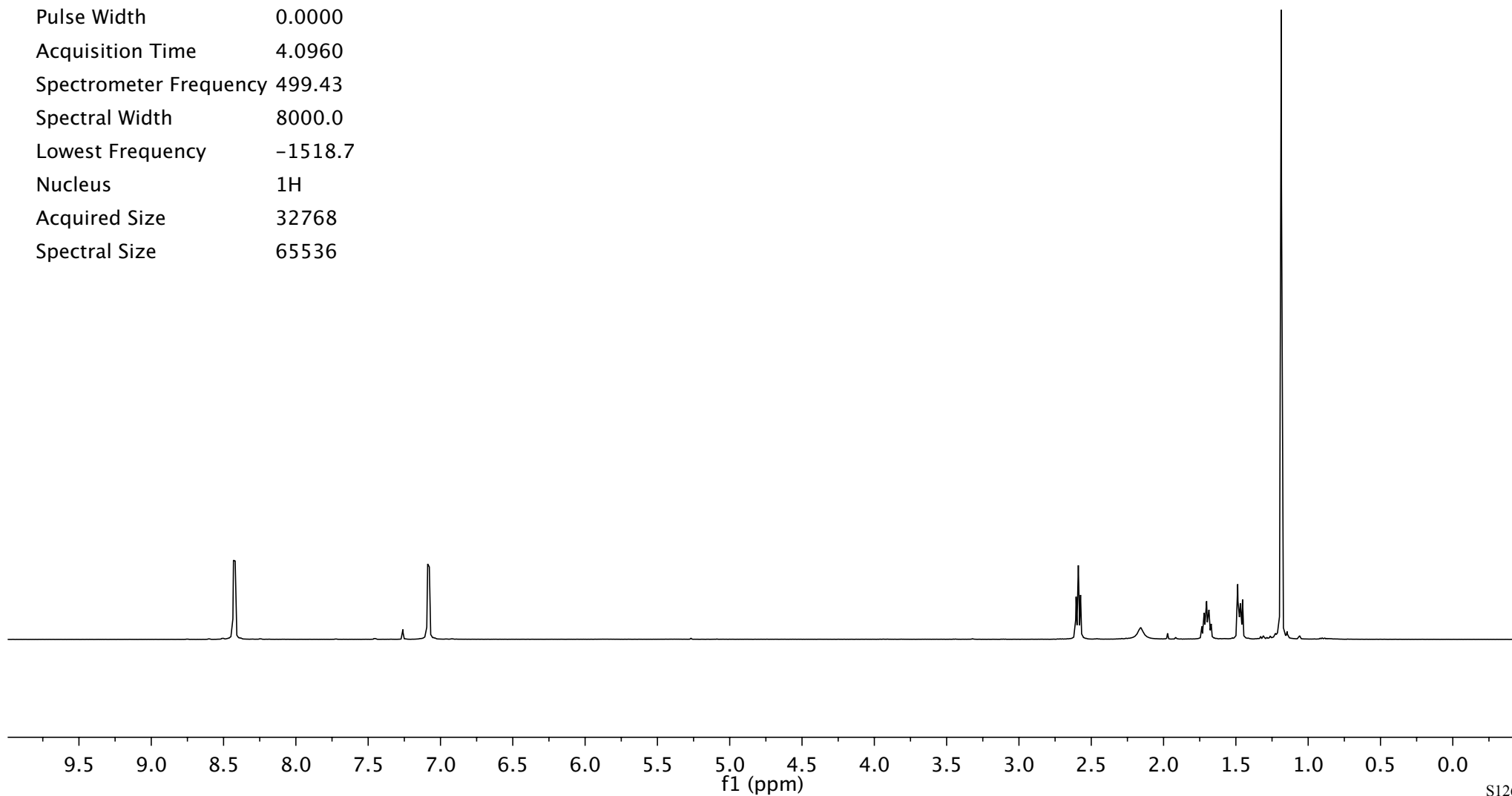
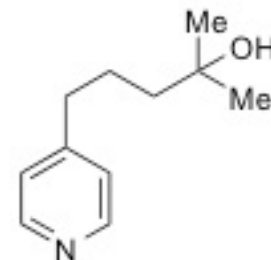


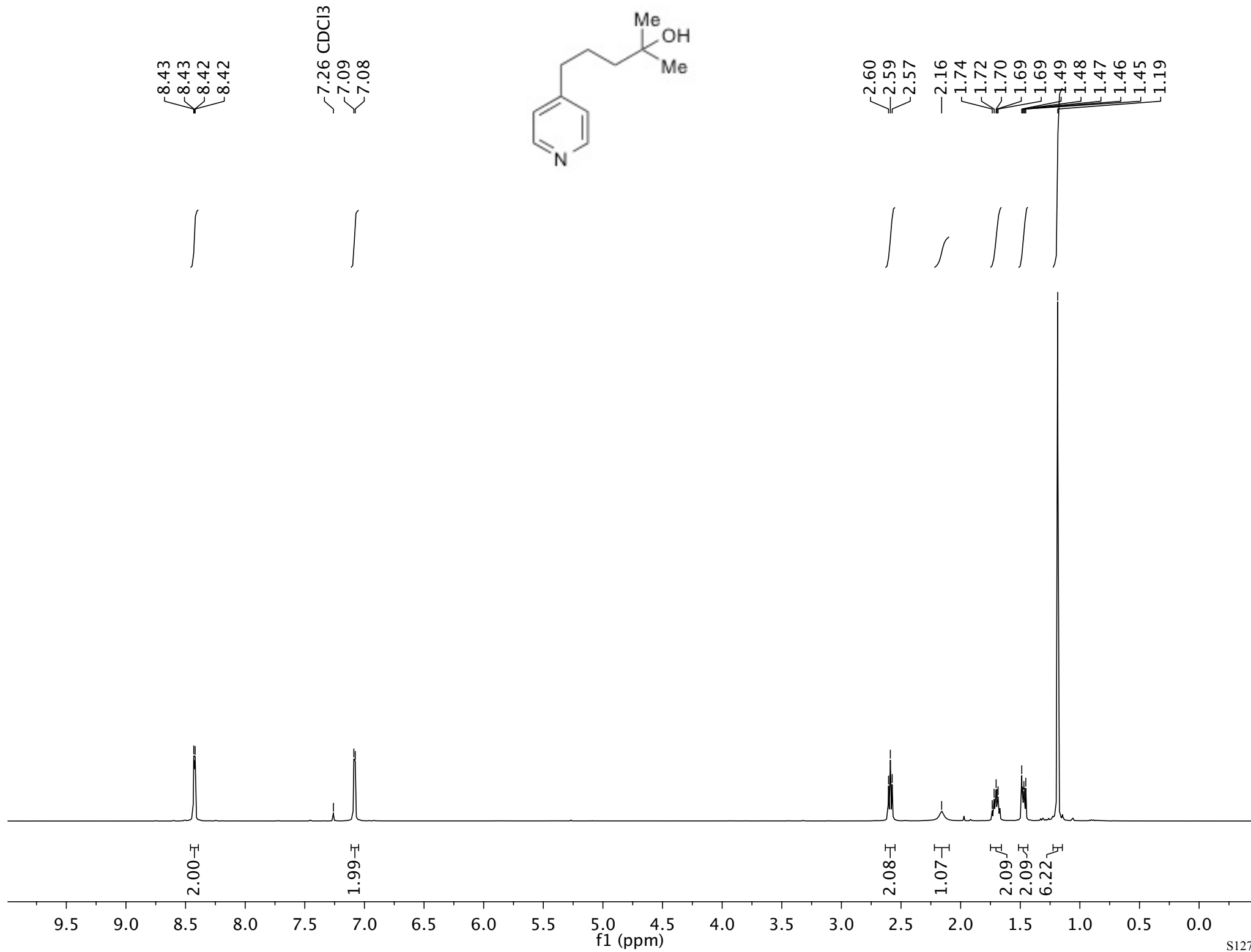


—71.10
—56.16
~46.59
~44.25
~37.16
~35.23
~32.54
~29.38
—21.64

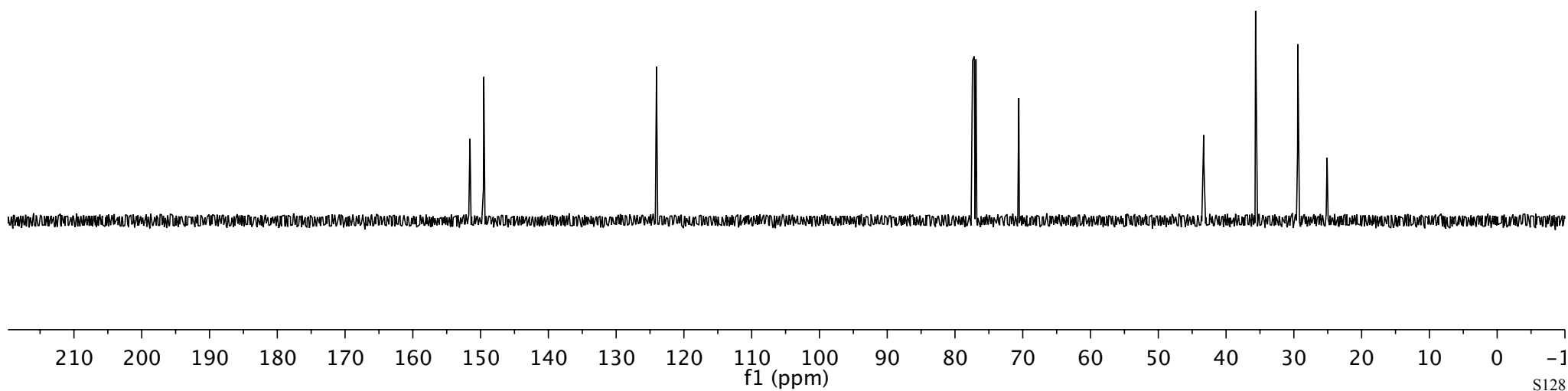
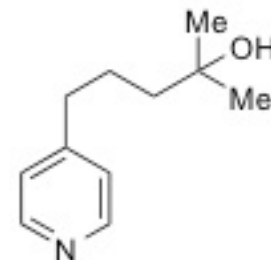


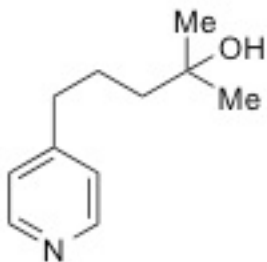
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	50
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	499.43
Spectral Width	8000.0
Lowest Frequency	-1518.7
Nucleus	1H
Acquired Size	32768
Spectral Size	65536





Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2208.6
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536





~151.57
~149.55

—124.02

—77.16 CDCl₃

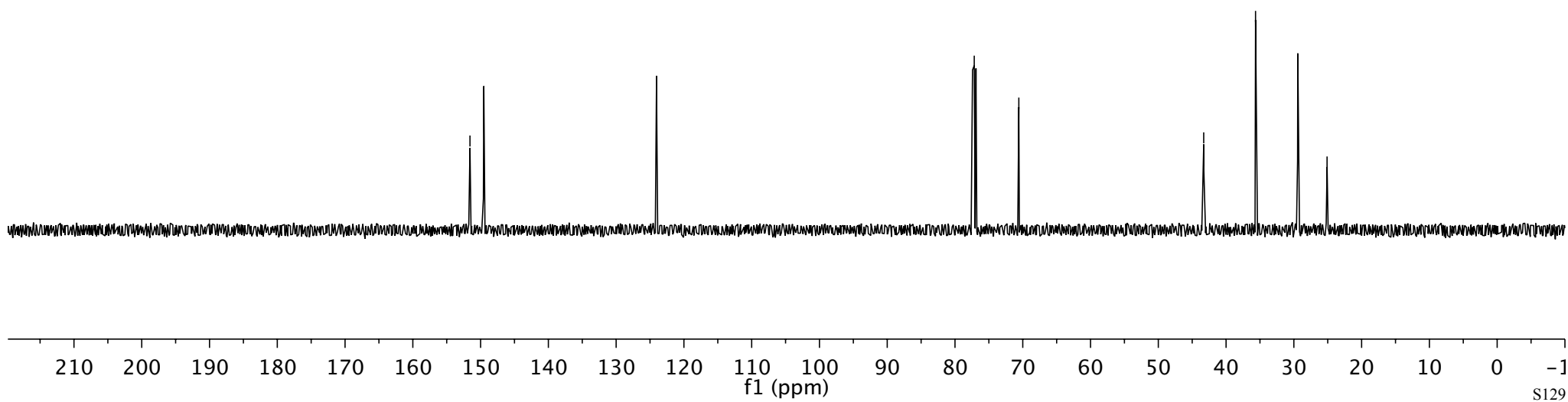
—70.58

—43.30

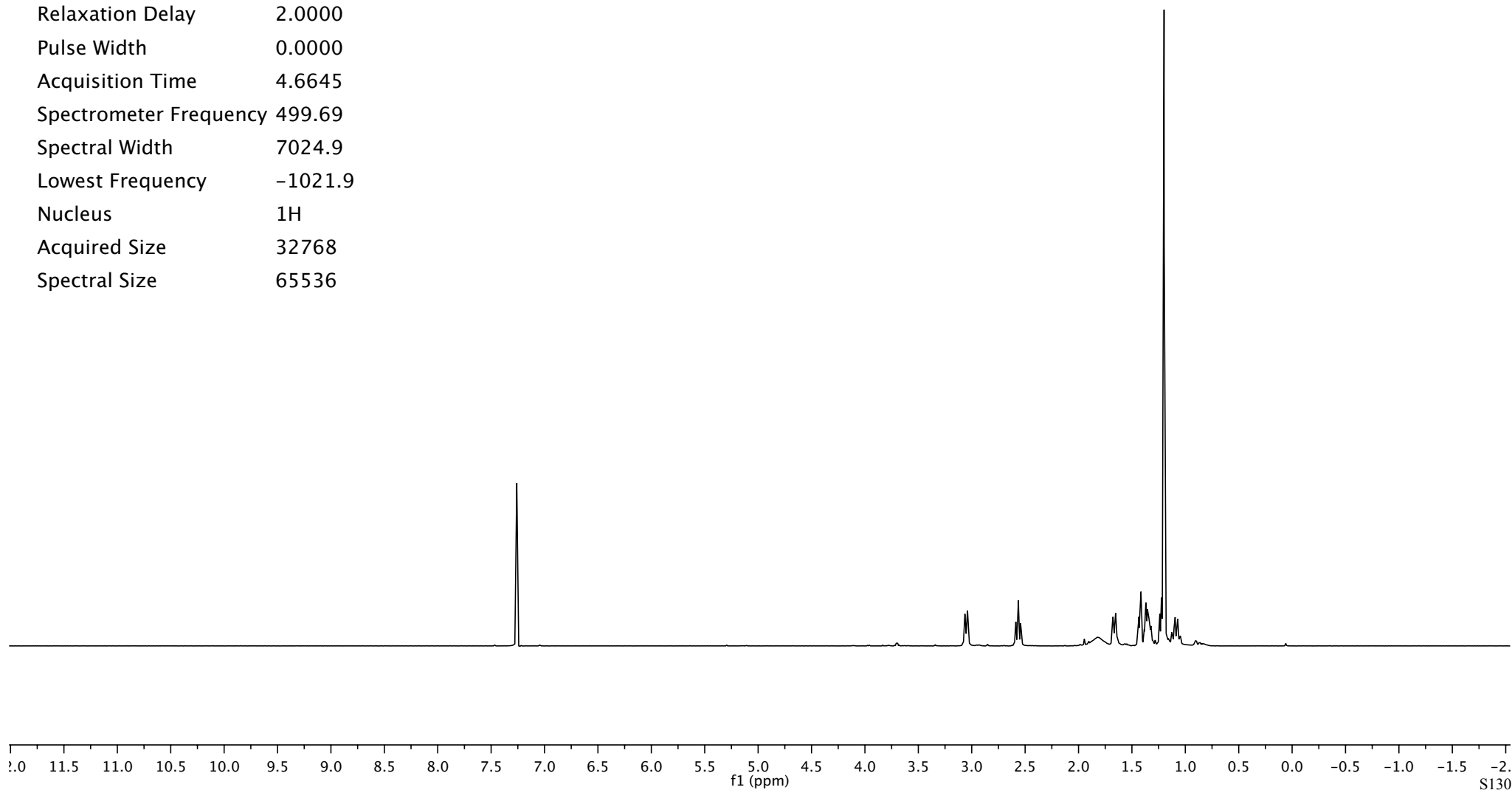
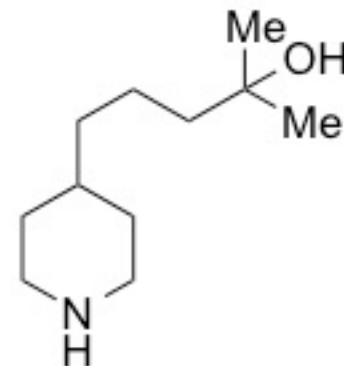
~35.65

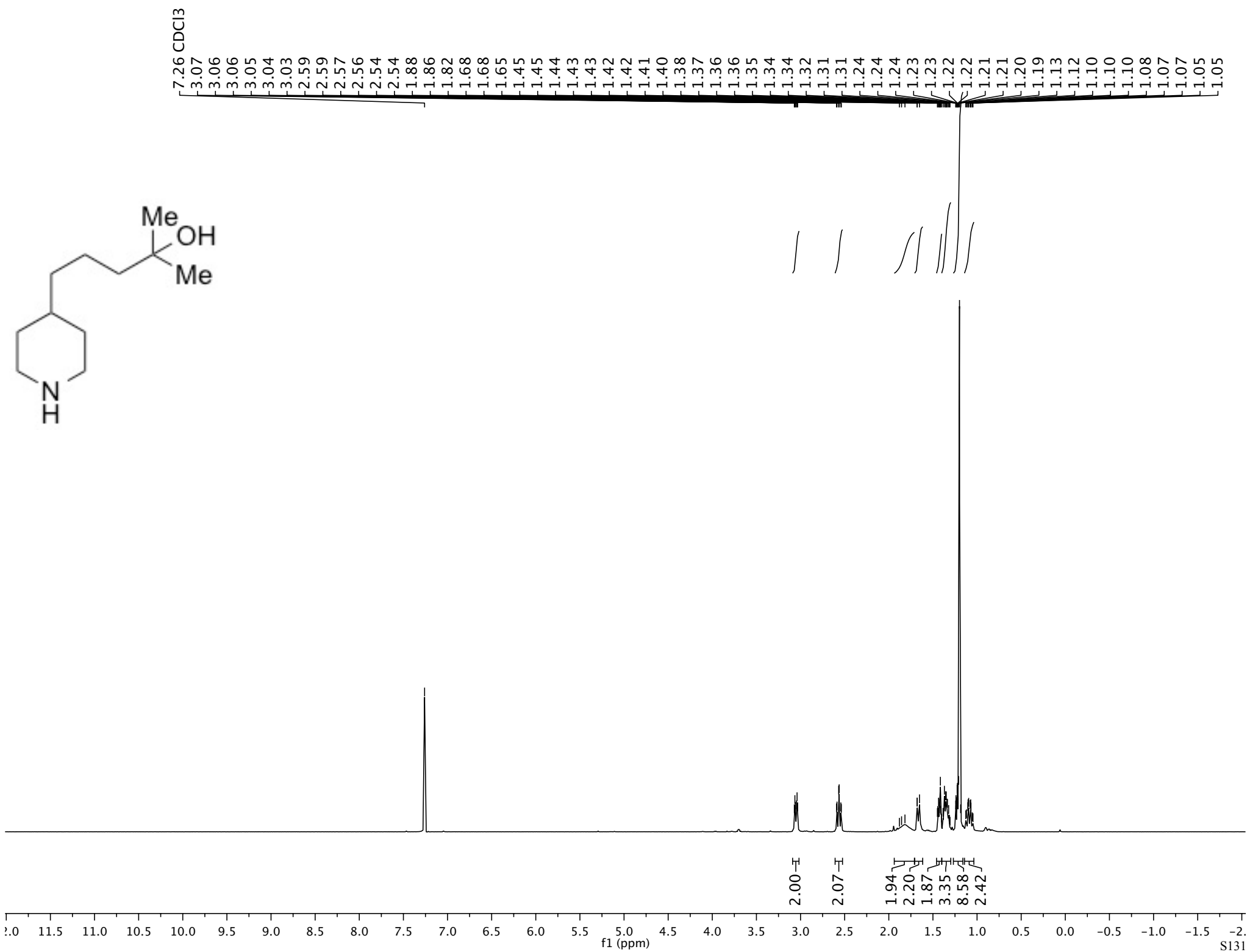
~29.40

~25.10

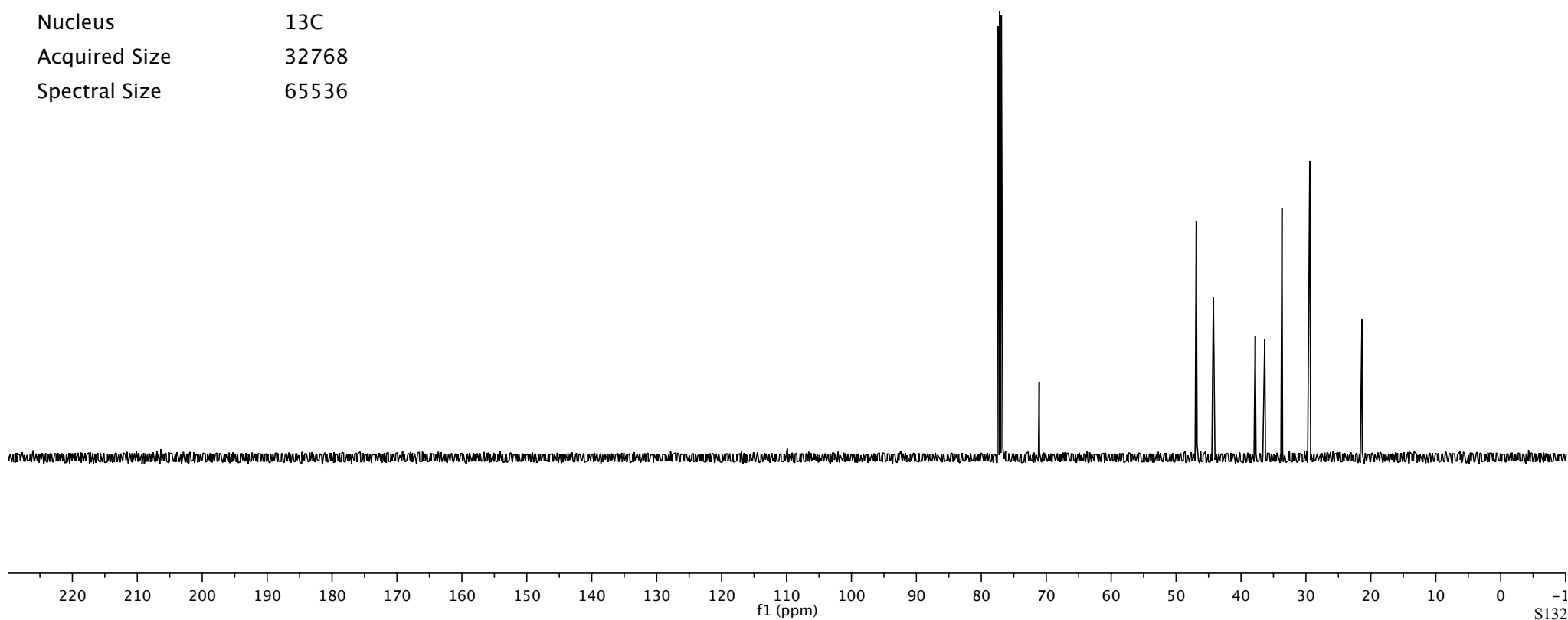
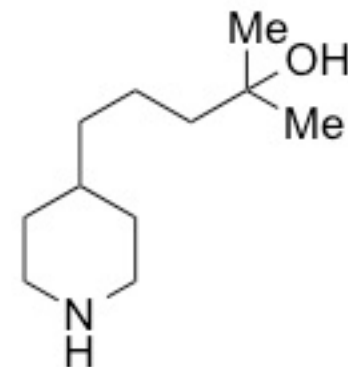


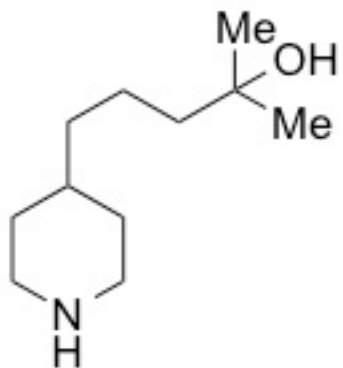
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	16
Receiver Gain	46
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.69
Spectral Width	7024.9
Lowest Frequency	-1021.9
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536





Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	611
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1273.1
Nucleus	13C
Acquired Size	32768
Spectral Size	65536





—77.16 CDCl₃

—71.09

—46.89

—44.26

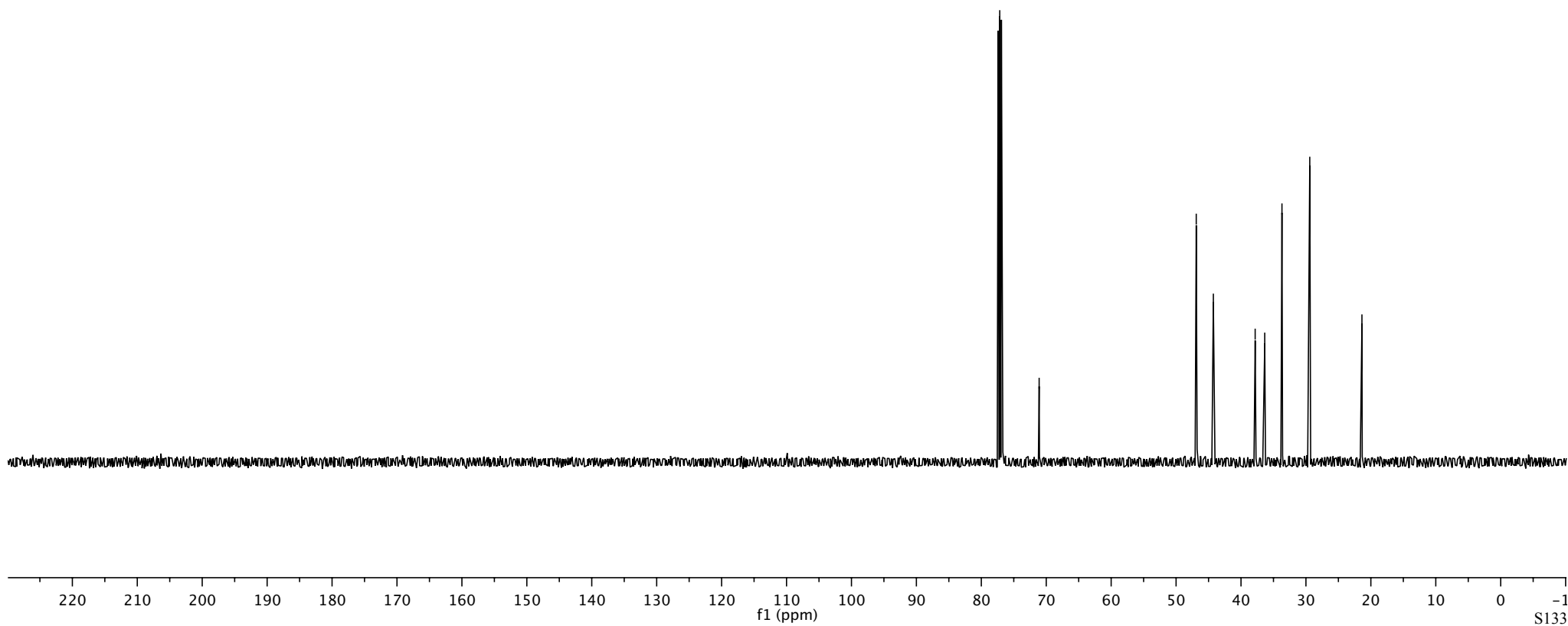
—37.82

—36.35

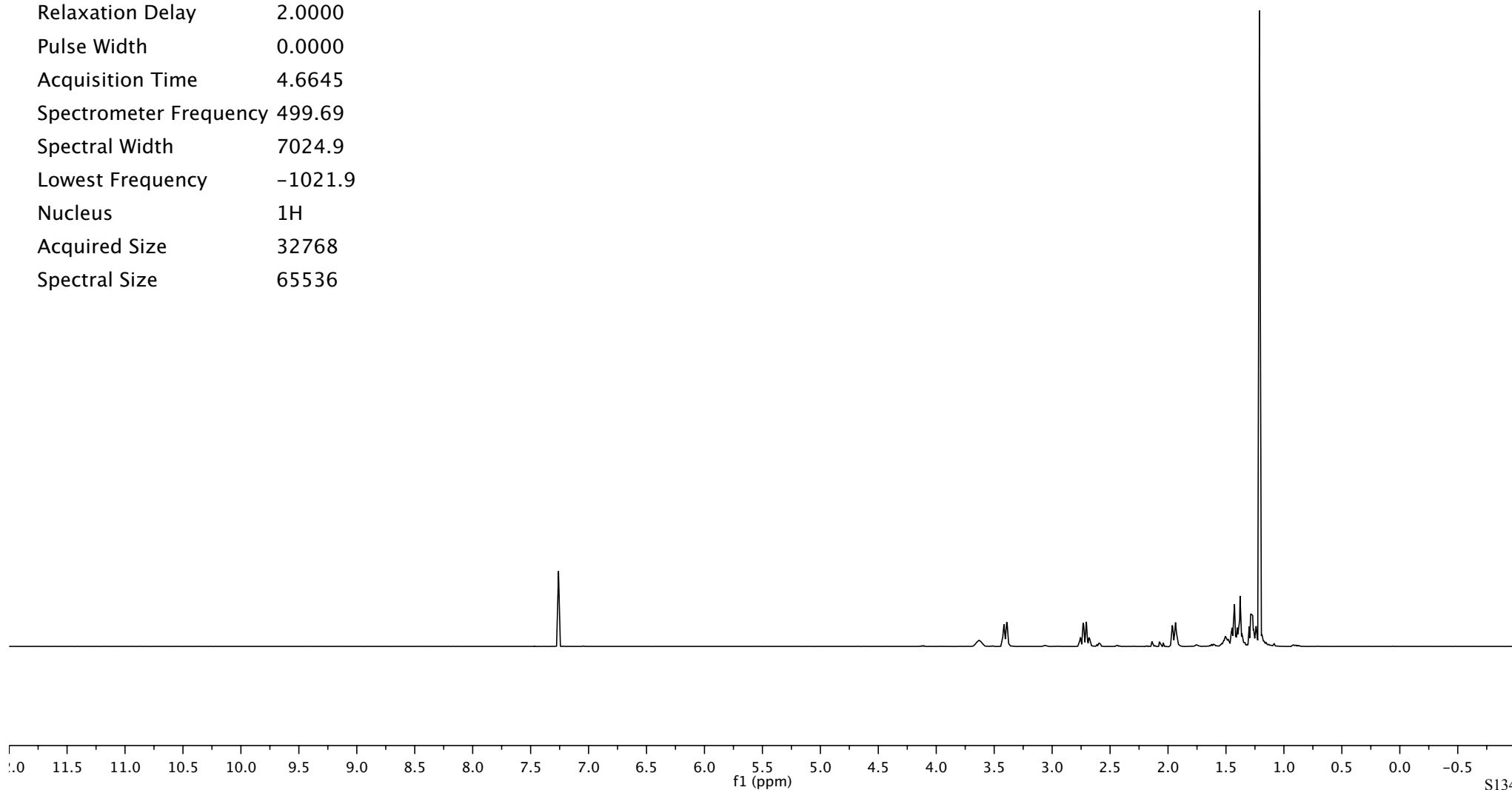
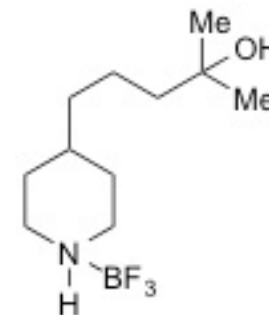
—33.69

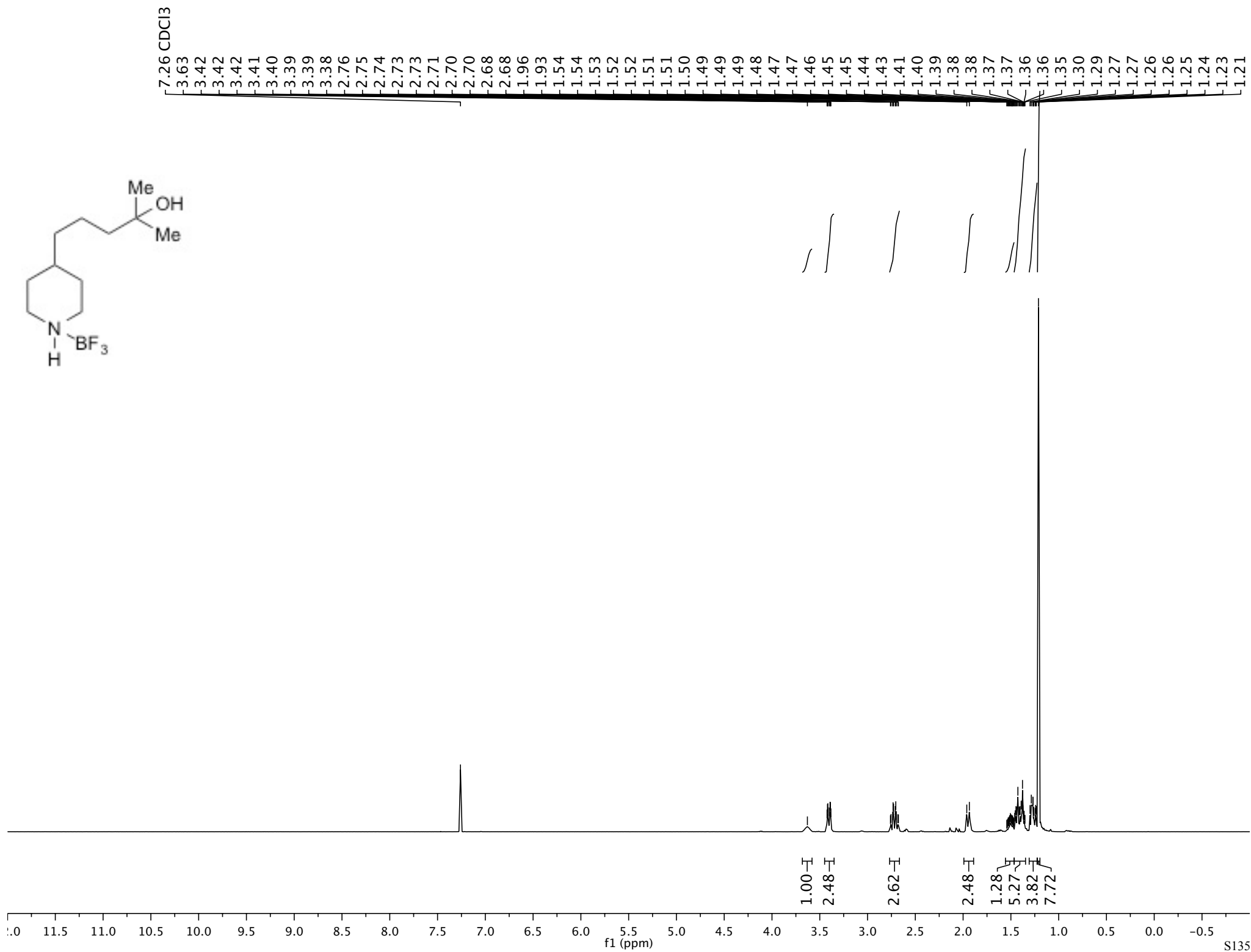
—29.41

—21.37

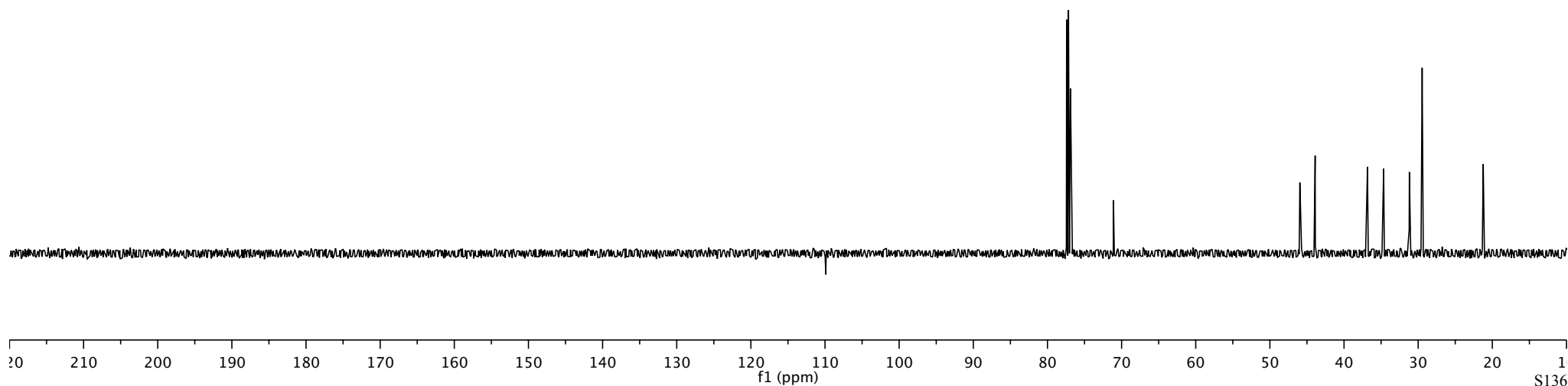
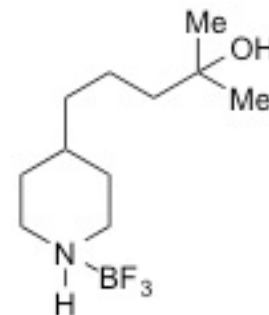


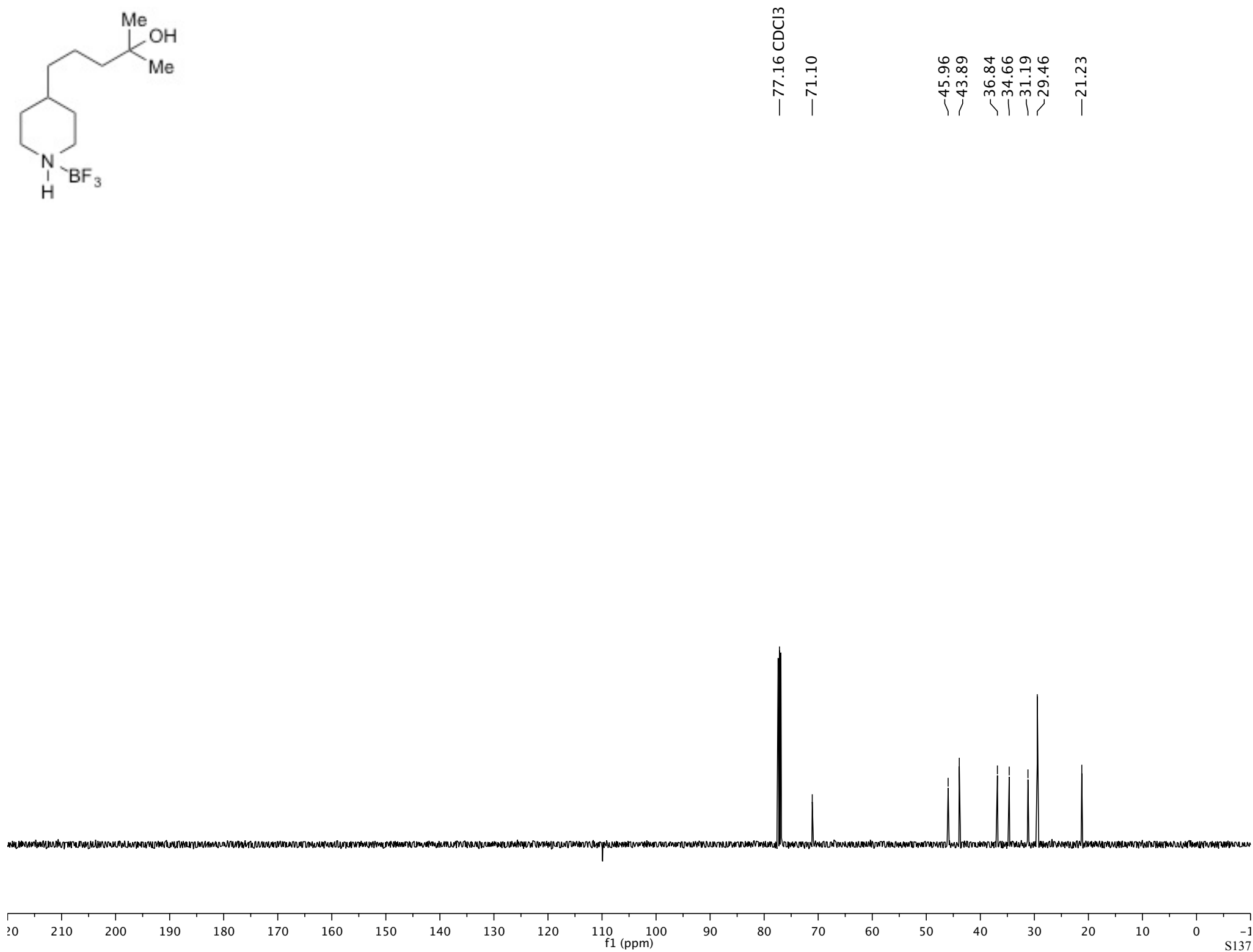
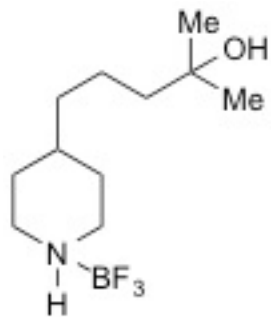
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	16
Receiver Gain	48
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.69
Spectral Width	7024.9
Lowest Frequency	-1021.9
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



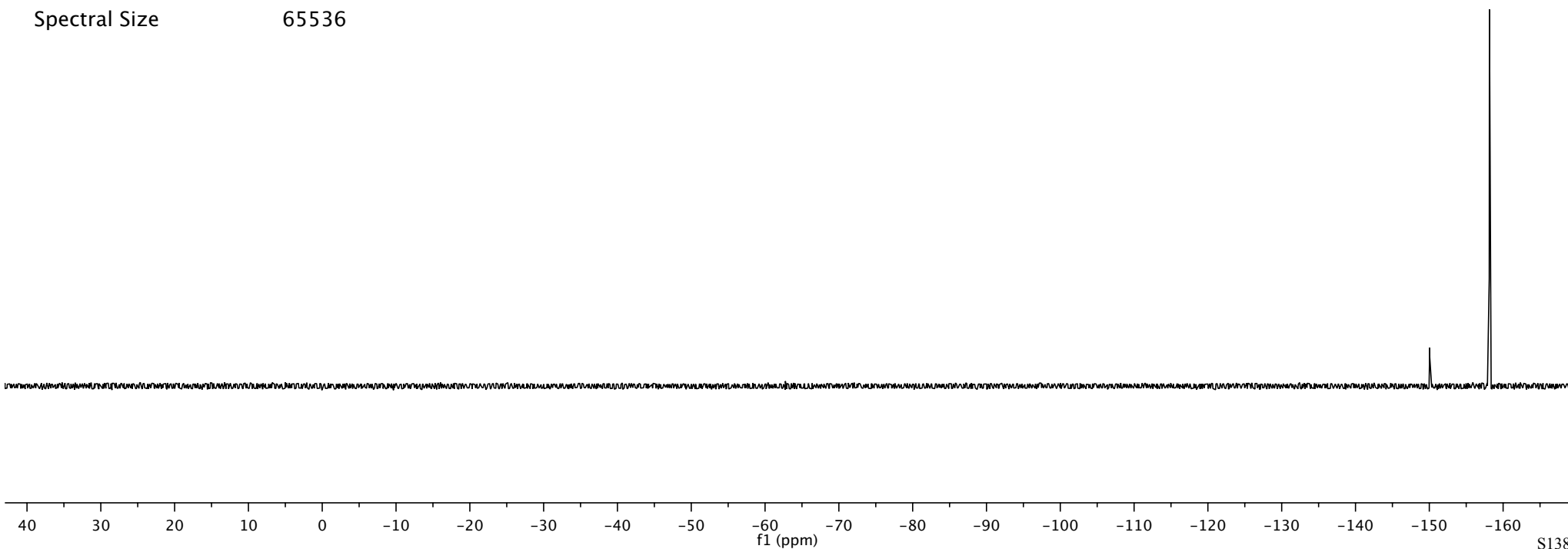
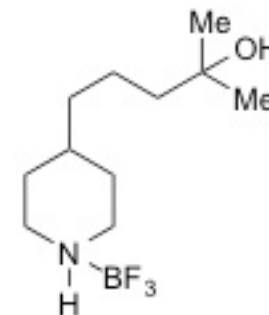


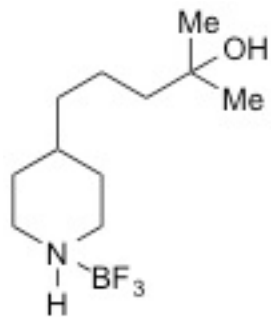
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	643
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1273.0
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



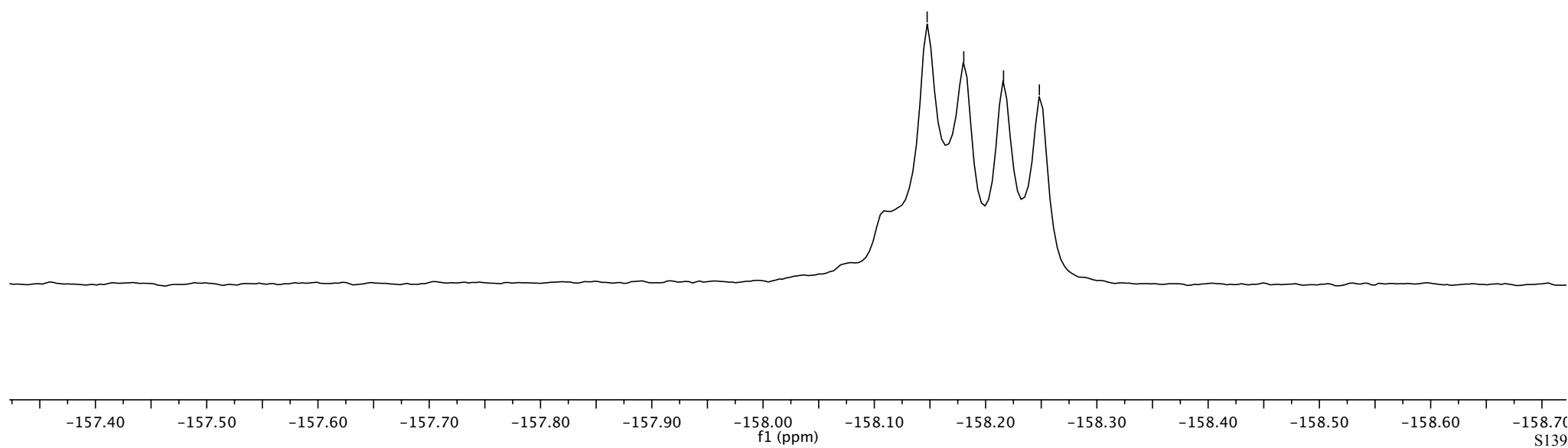


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	132
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency	-79501.3
Nucleus	¹⁹ F
Acquired Size	32768
Spectral Size	65536

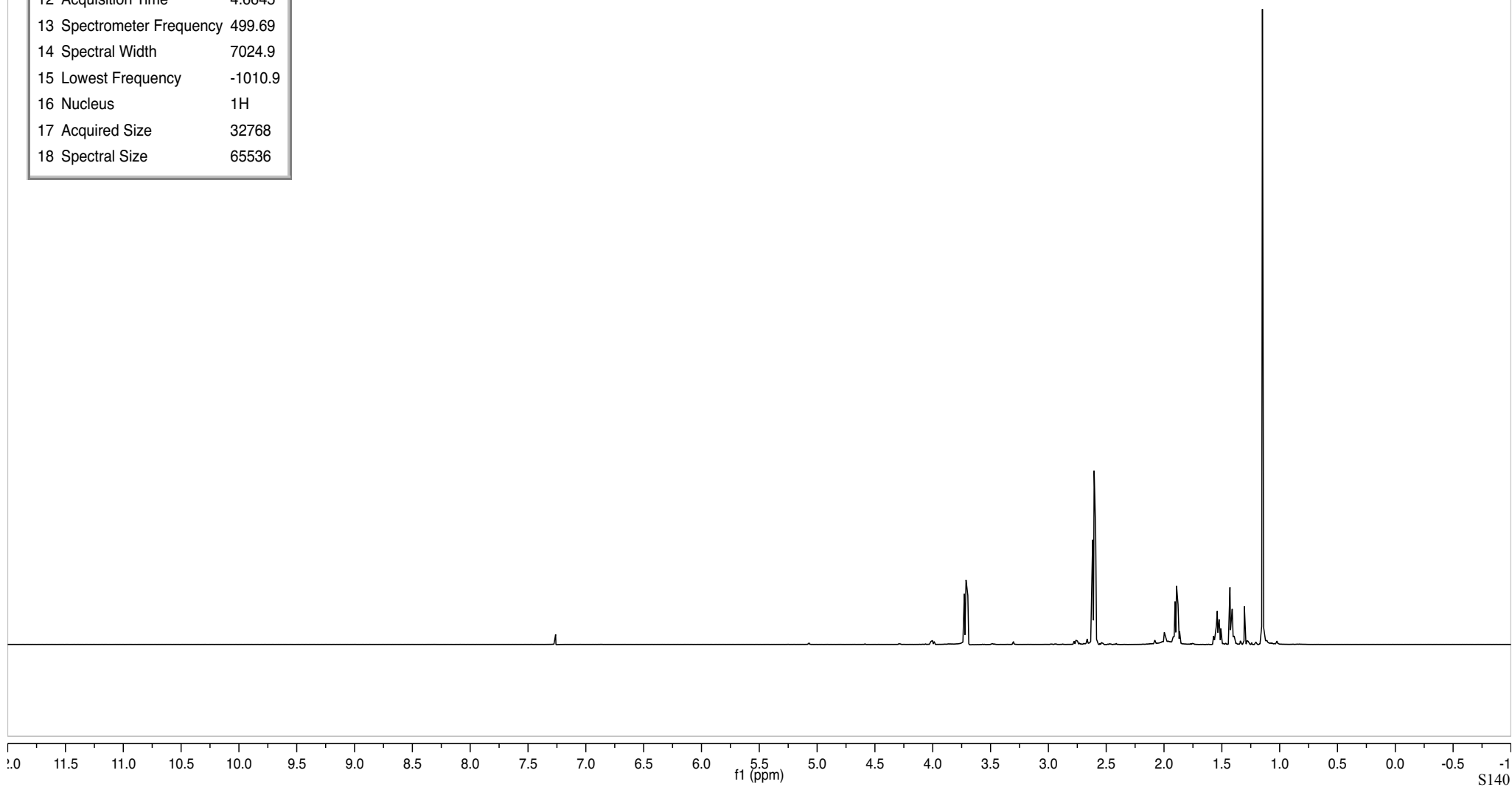
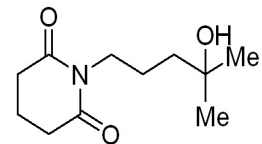


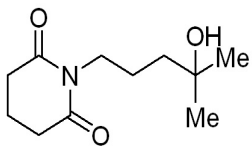


158.15
158.18
158.22
158.25

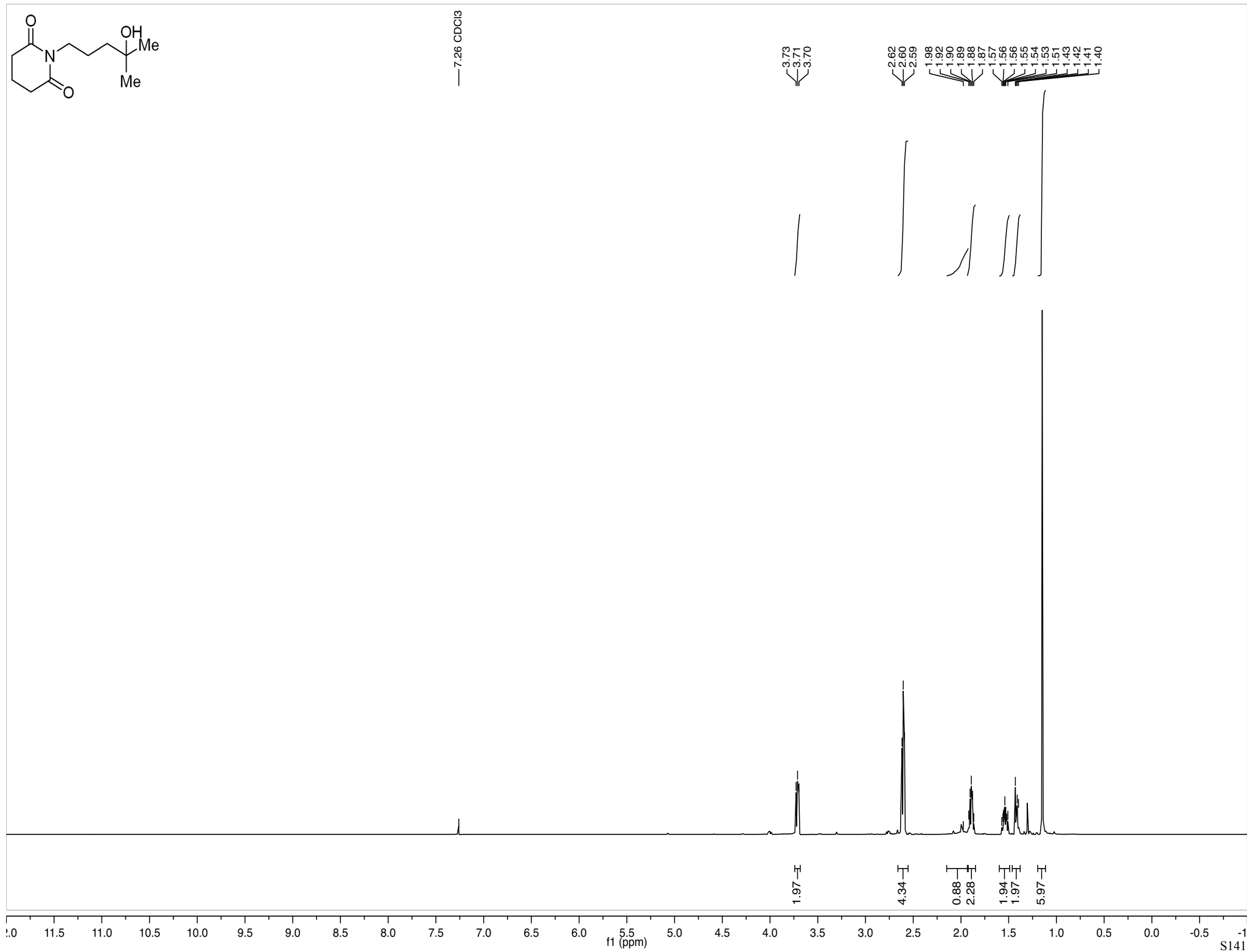


	Parameter	Value
1	Origin	Varian
2	Spectrometer	inova
3	Solvent	CDCl3
4	Temperature	20.0
5	Pulse Sequence	s2pul
6	Experiment	1D
7	Probe	QUAD
8	Number of Scans	8
9	Receiver Gain	36
10	Relaxation Delay	0.0000
11	Pulse Width	0.0000
12	Acquisition Time	4.6645
13	Spectrometer Frequency	499.69
14	Spectral Width	7024.9
15	Lowest Frequency	-1010.9
16	Nucleus	¹ H
17	Acquired Size	32768
18	Spectral Size	65536

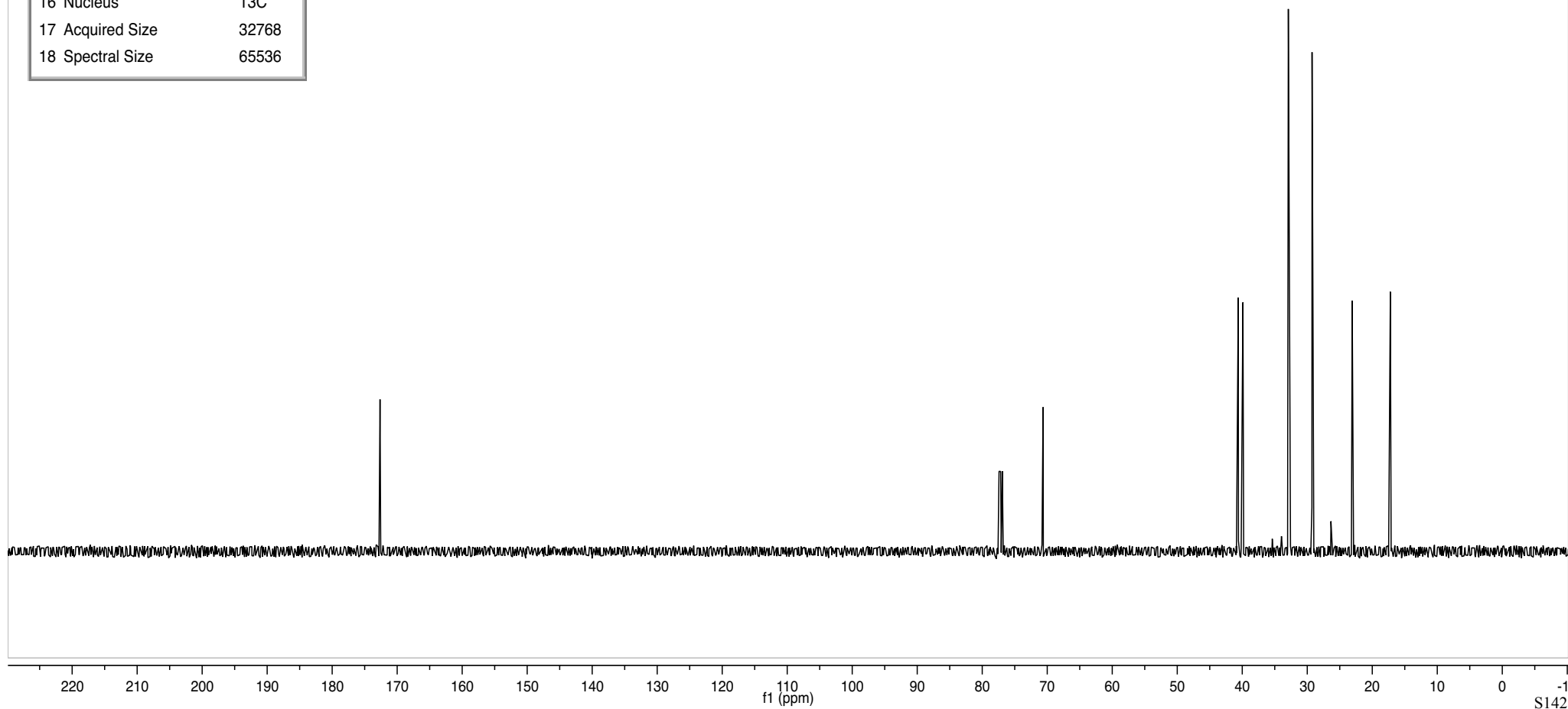
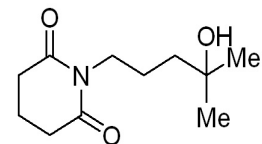


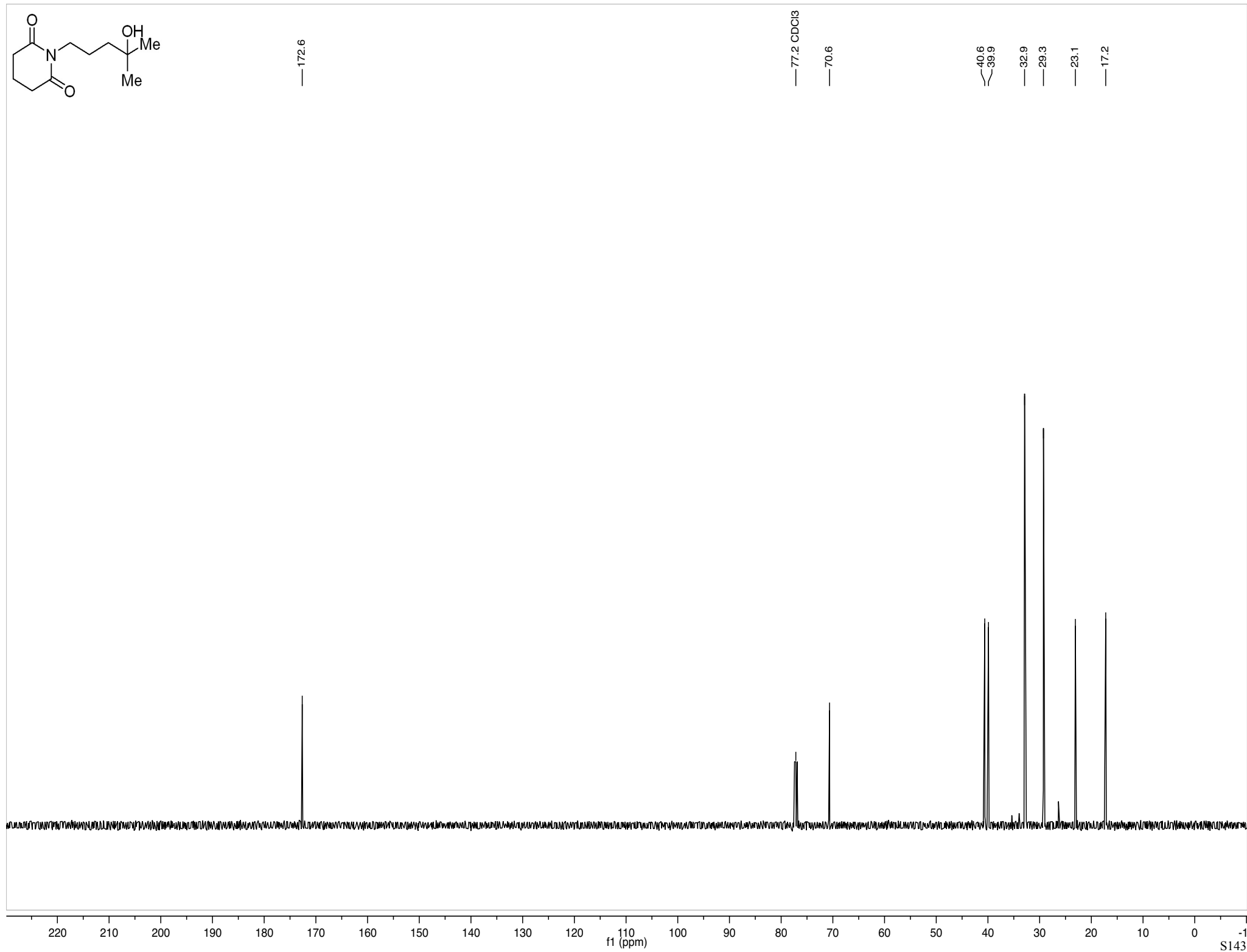
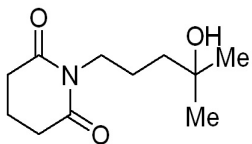


— 7.26 CDCl₃

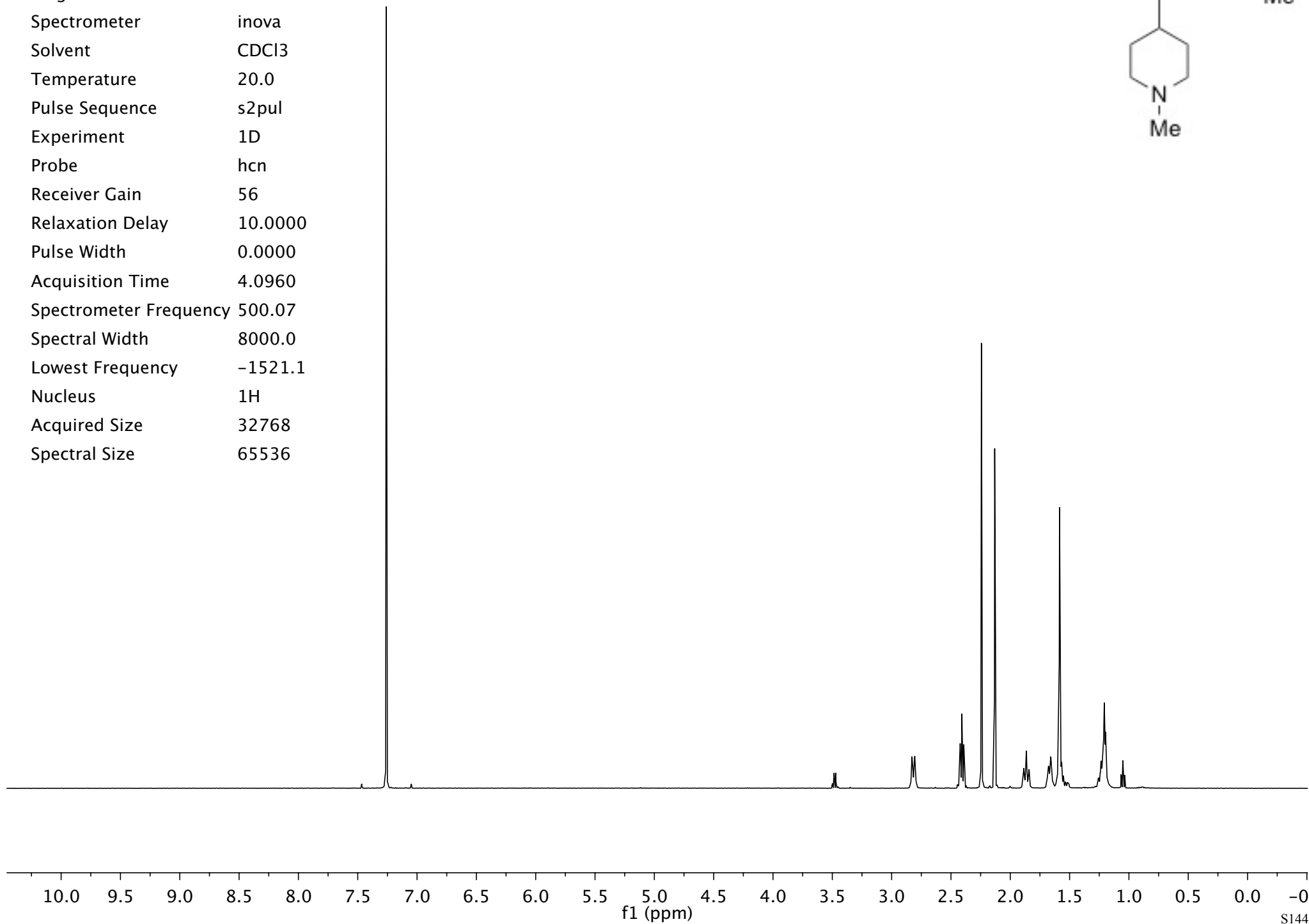
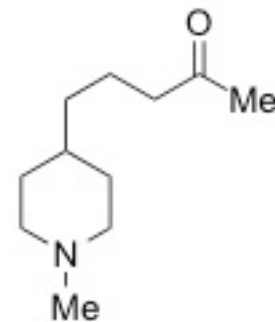


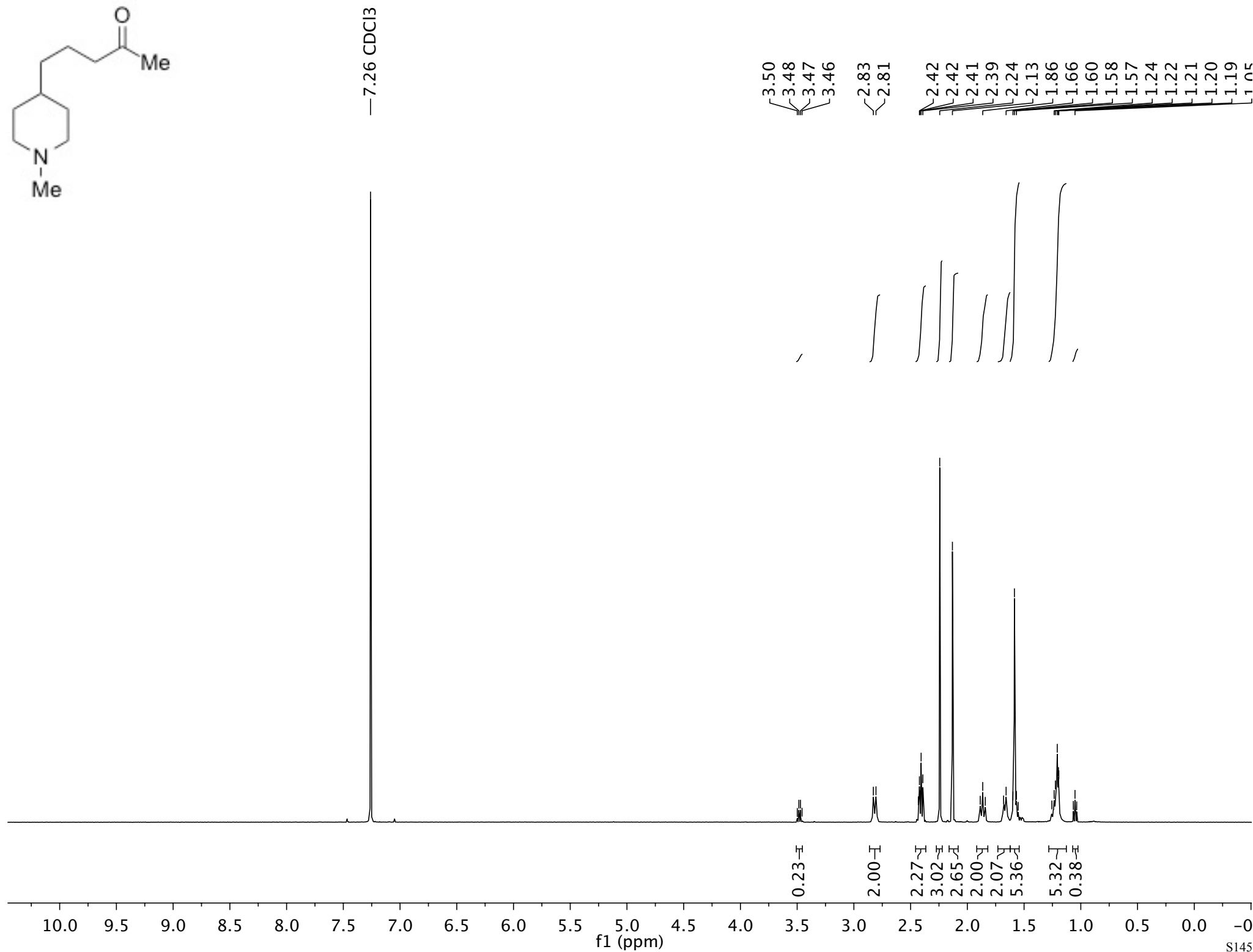
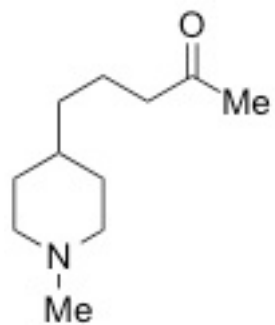
	Parameter	Value
1	Origin	Varian
2	Spectrometer	inova
3	Solvent	CDCl3
4	Temperature	20.0
5	Pulse Sequence	s2pul
6	Experiment	1D
7	Probe	QUAD
8	Number of Scans	48
9	Receiver Gain	60
10	Relaxation Delay	1.0000
11	Pulse Width	0.0000
12	Acquisition Time	1.0863
13	Spectrometer Frequency	125.66
14	Spectral Width	30165.9
15	Lowest Frequency	-1279.2
16	Nucleus	¹³ C
17	Acquired Size	32768
18	Spectral Size	65536



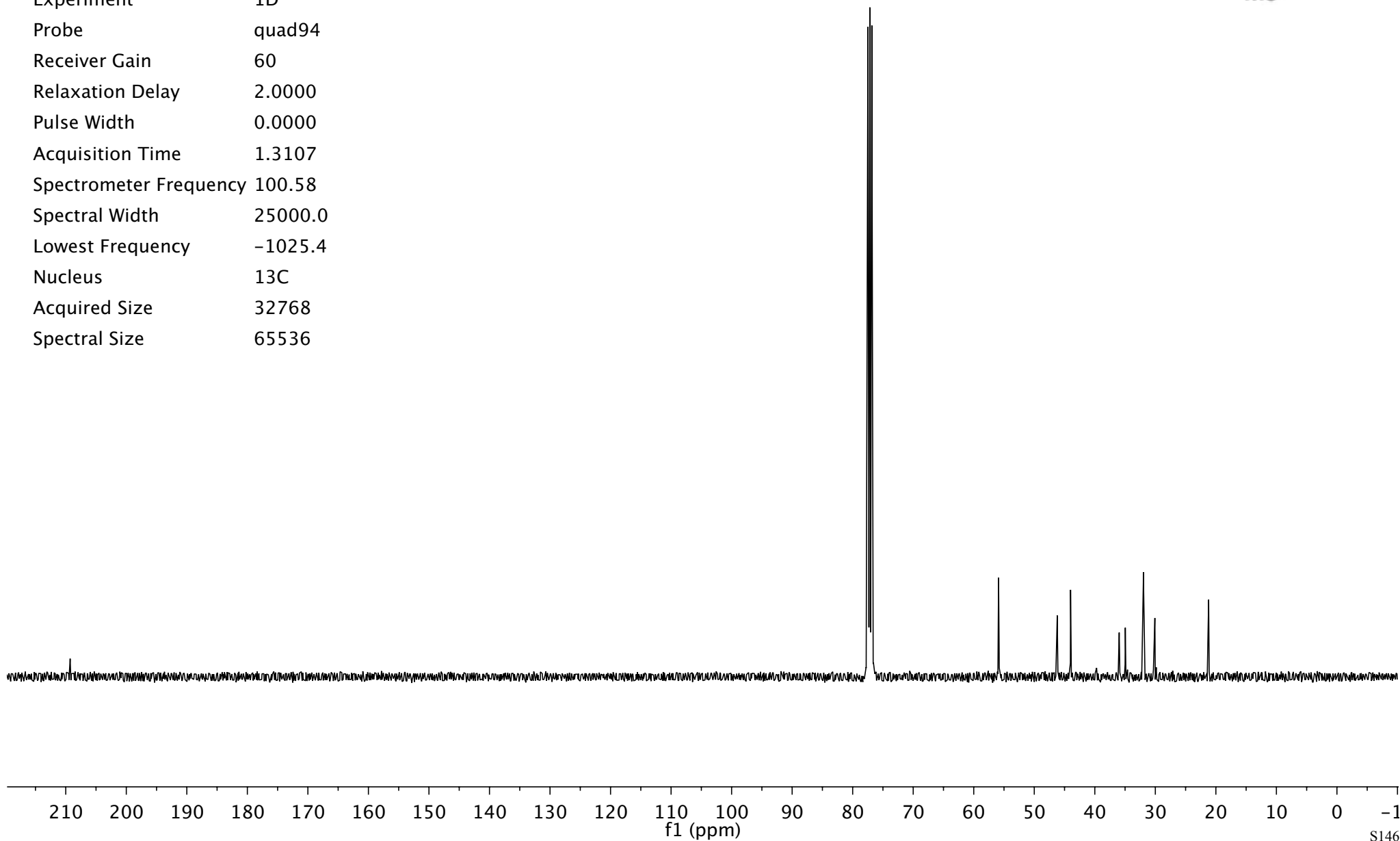
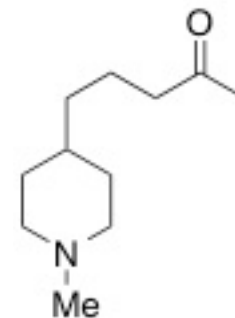


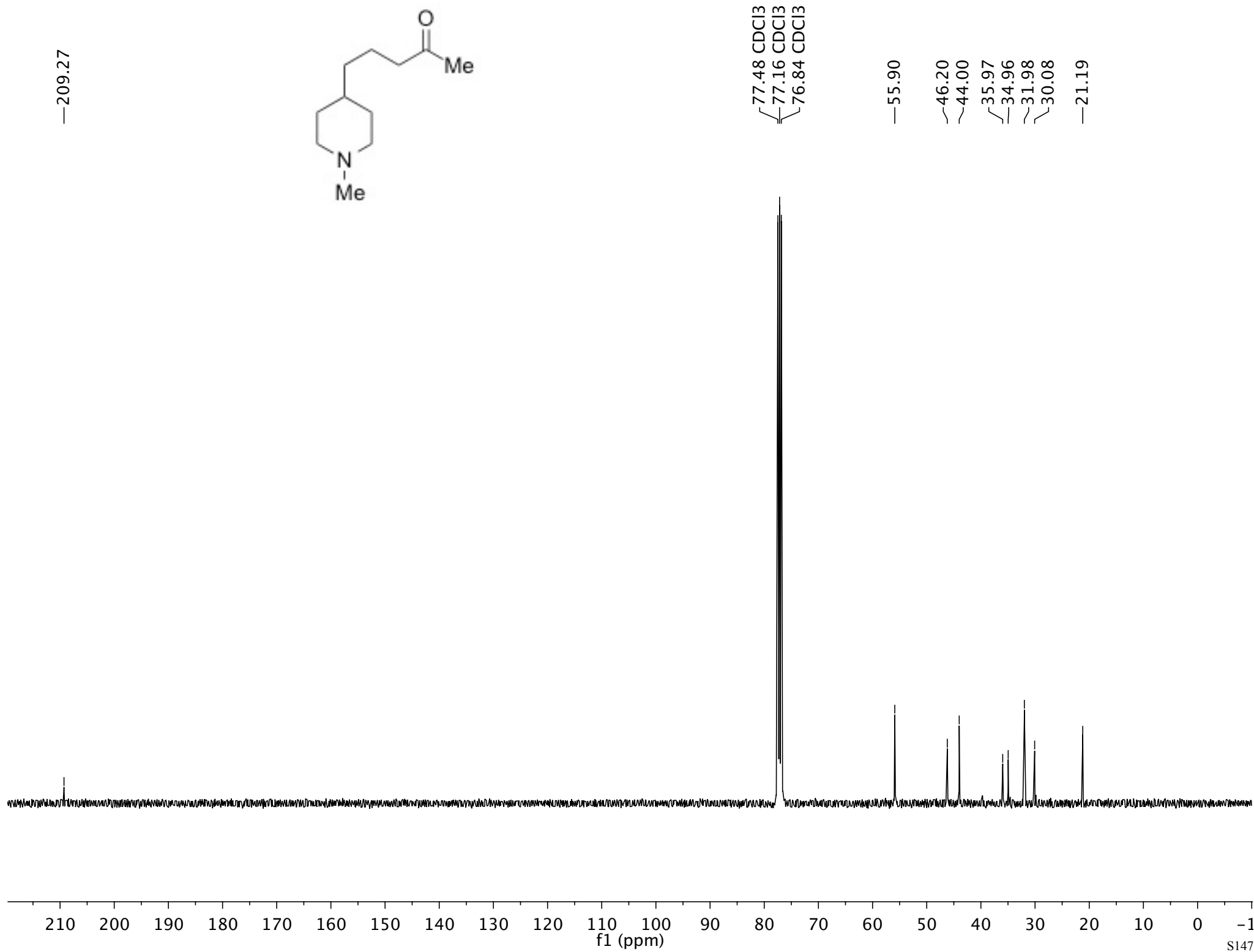
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	56
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



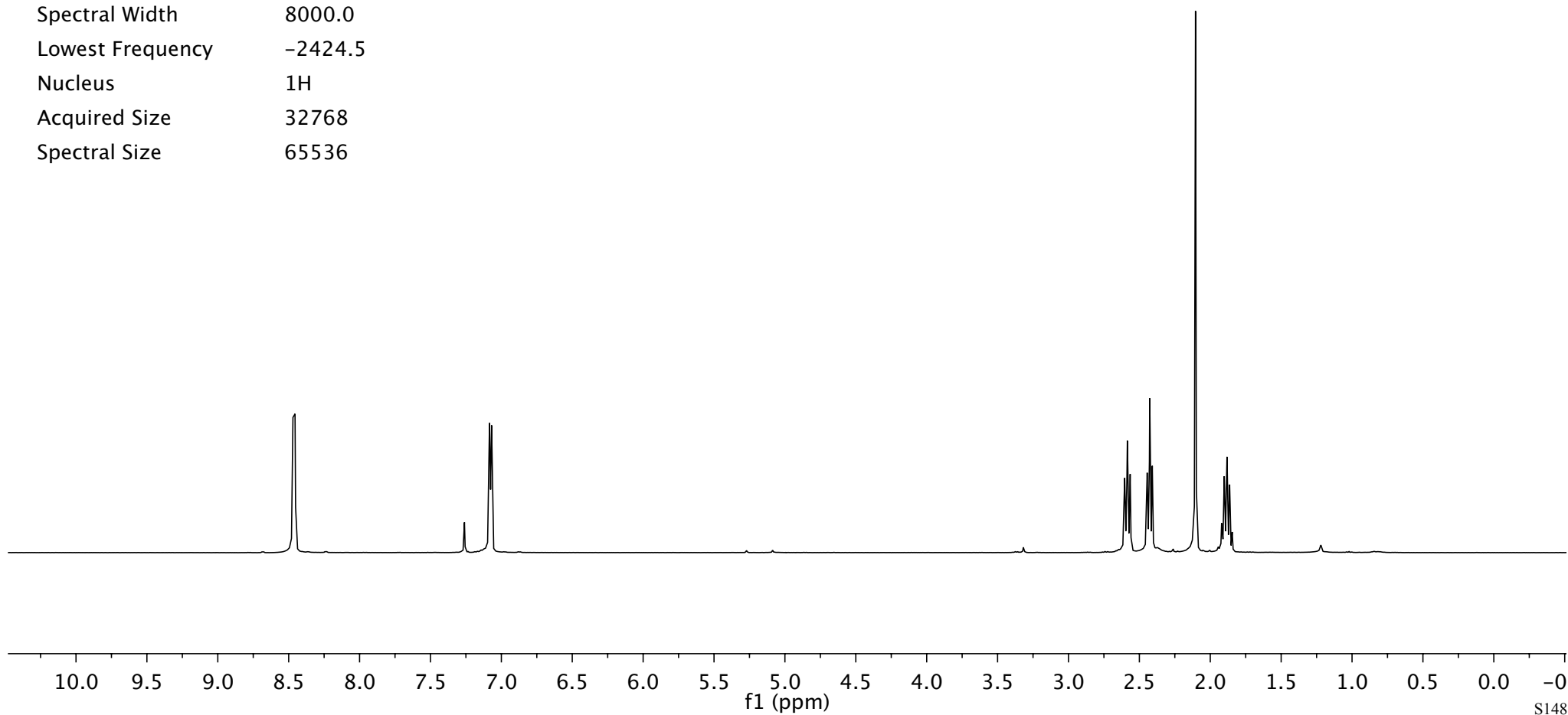
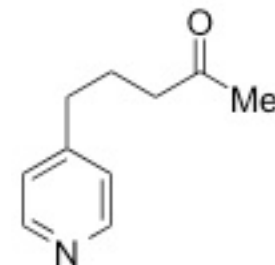


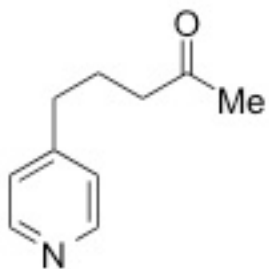
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.3107
Spectrometer Frequency	100.58
Spectral Width	25000.0
Lowest Frequency	-1025.4
Nucleus	13C
Acquired Size	32768
Spectral Size	65536





Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	46
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	399.95
Spectral Width	8000.0
Lowest Frequency	-2424.5
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536





8.47
8.47
8.46
8.46

7.26 CDCl₃

7.08
7.07

2.60
2.58
2.56
2.44
2.43
2.41
2.10
1.92
1.90
1.88
1.86
1.85



1.95

1.97

2.00

2.03

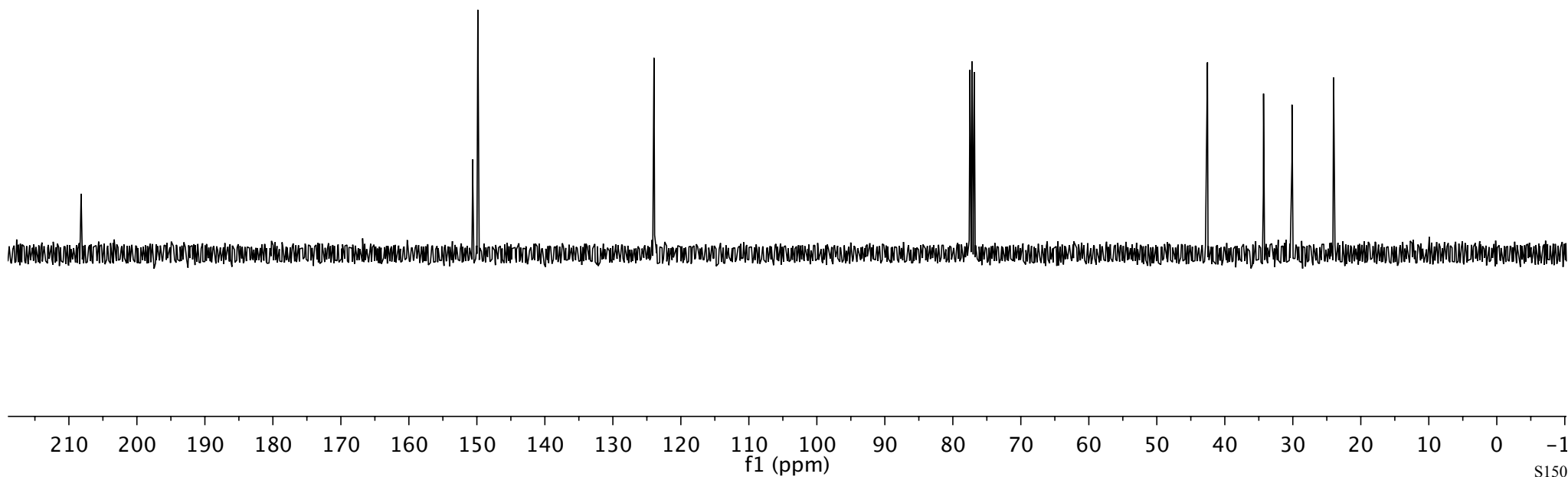
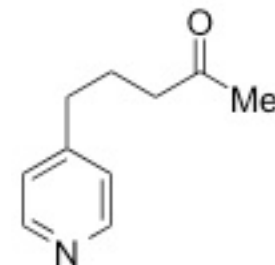
2.92

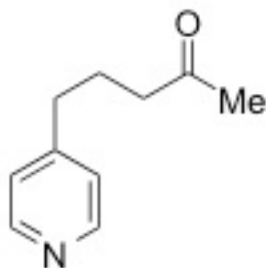
1.99

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0

f1 (ppm)

Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.3107
Spectrometer Frequency	100.58
Spectral Width	25000.0
Lowest Frequency	-1031.7
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536





—208.20

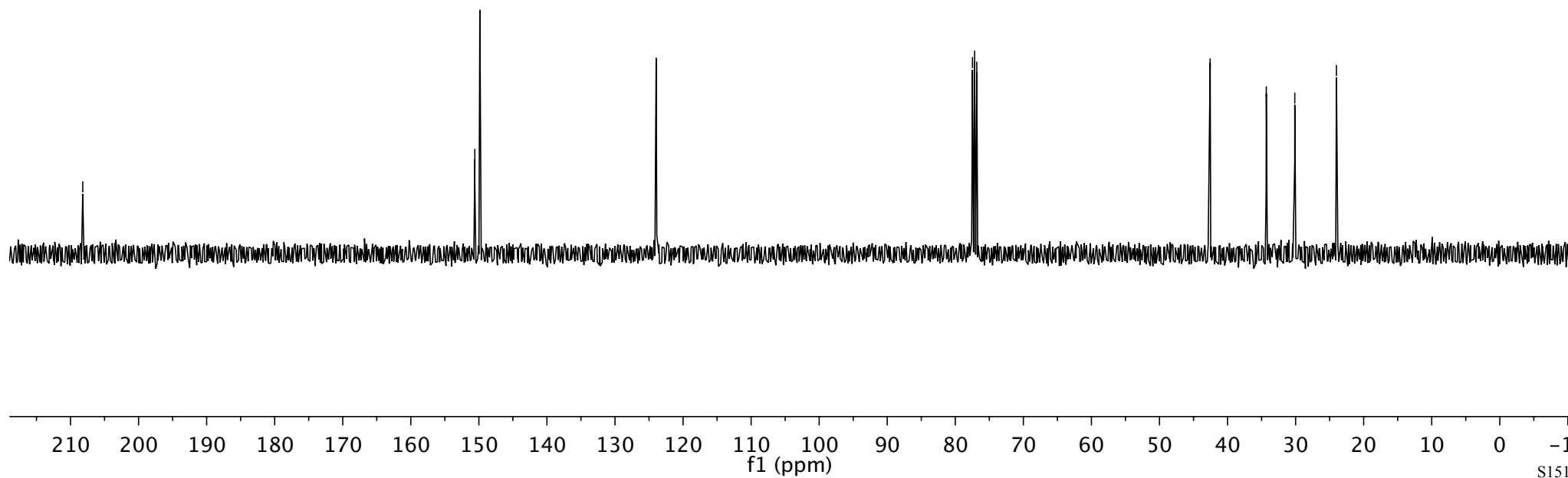
150.60
149.84

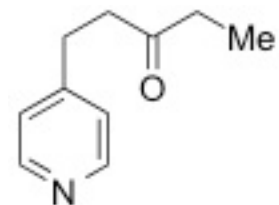
—123.94

77.48 CDCl3
77.16 CDCl3
76.84 CDCl3

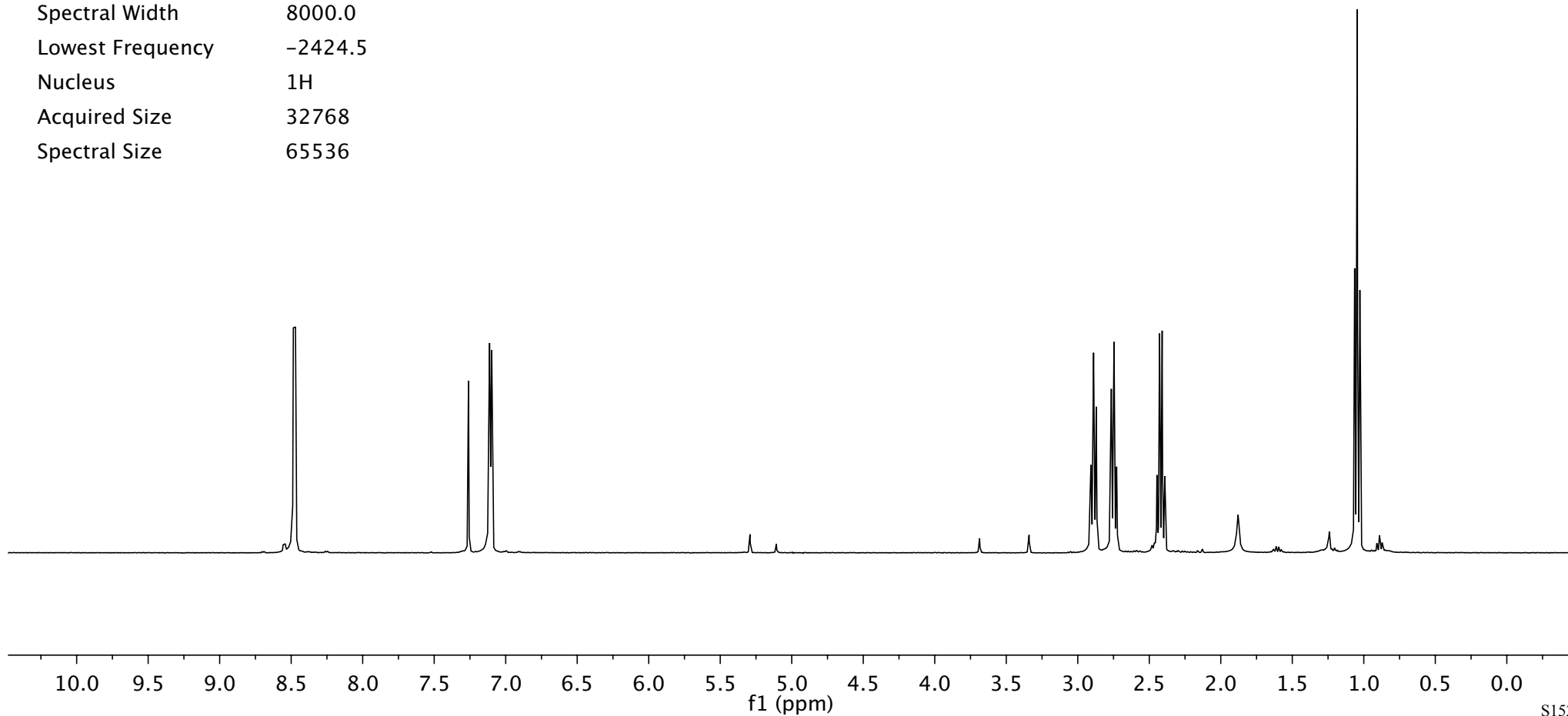
—42.56

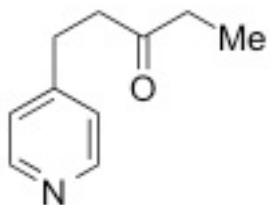
34.31
30.12
24.00





Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	58
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	399.95
Spectral Width	8000.0
Lowest Frequency	-2424.5
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



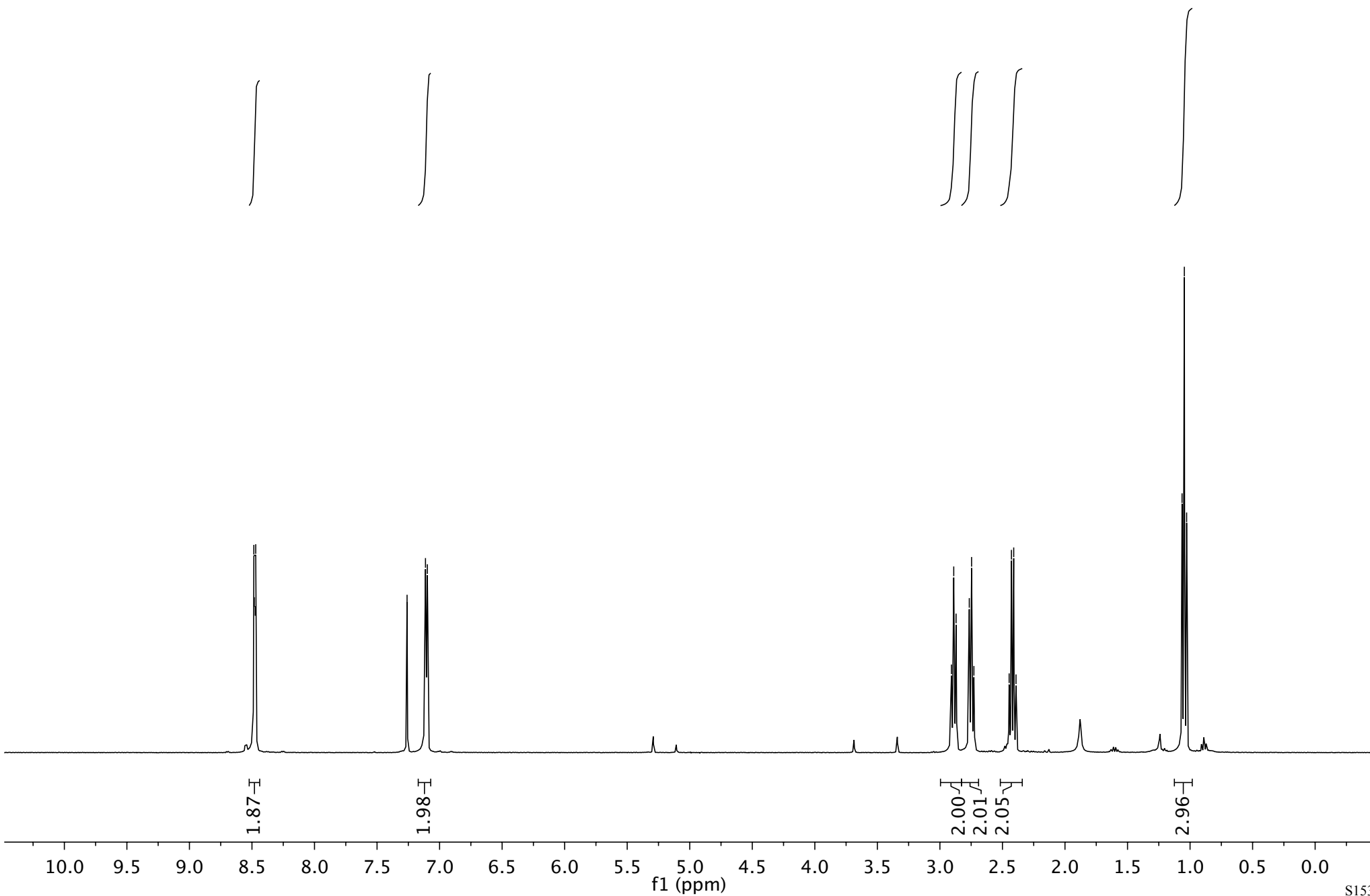


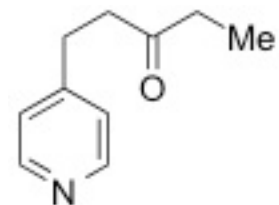
8.49
8.48
8.47
8.47

7.26 CDCl₃
7.11
7.10

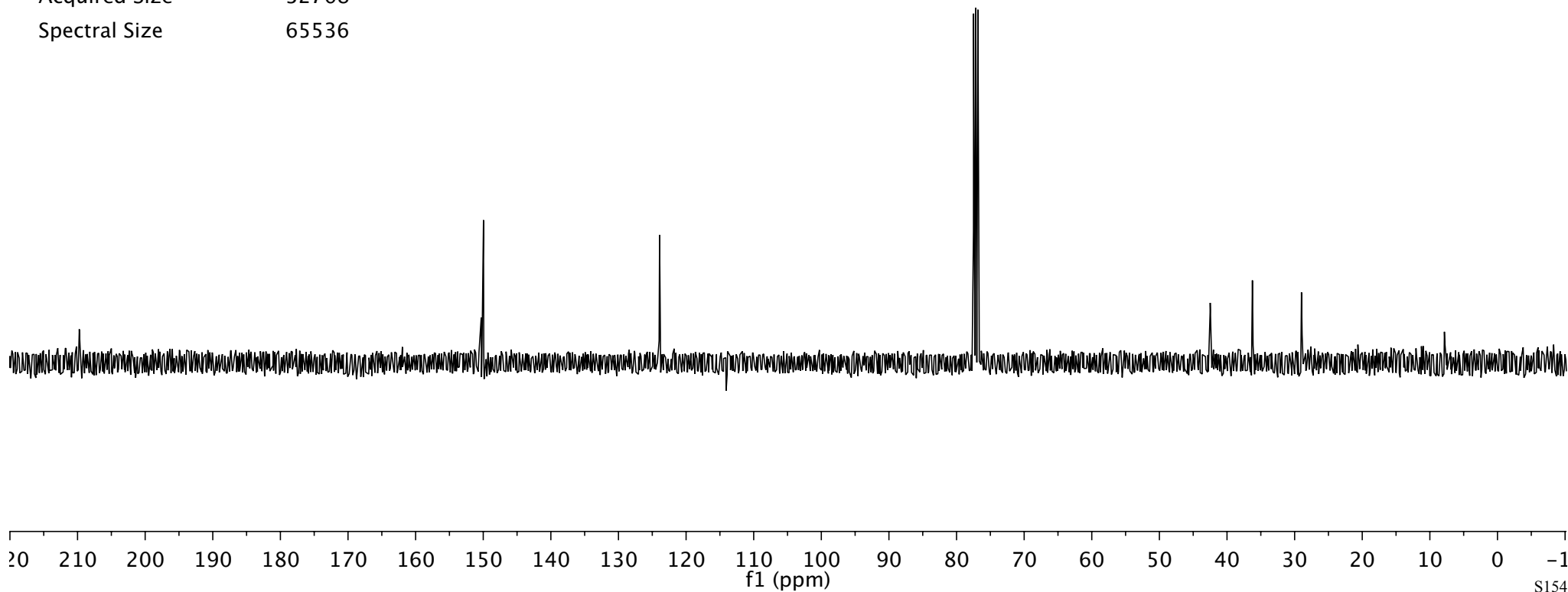
2.91
2.89
2.87
2.77
2.75
2.73
2.45
2.43
2.41
2.39

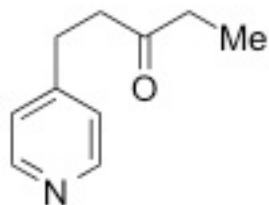
1.06
1.05
1.03





Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.3107
Spectrometer Frequency	100.58
Spectral Width	25000.0
Lowest Frequency	-1026.6
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536





—209.74

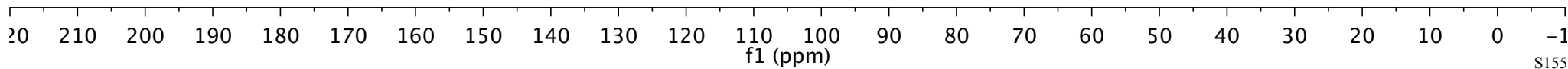
150.30
149.96

—123.92

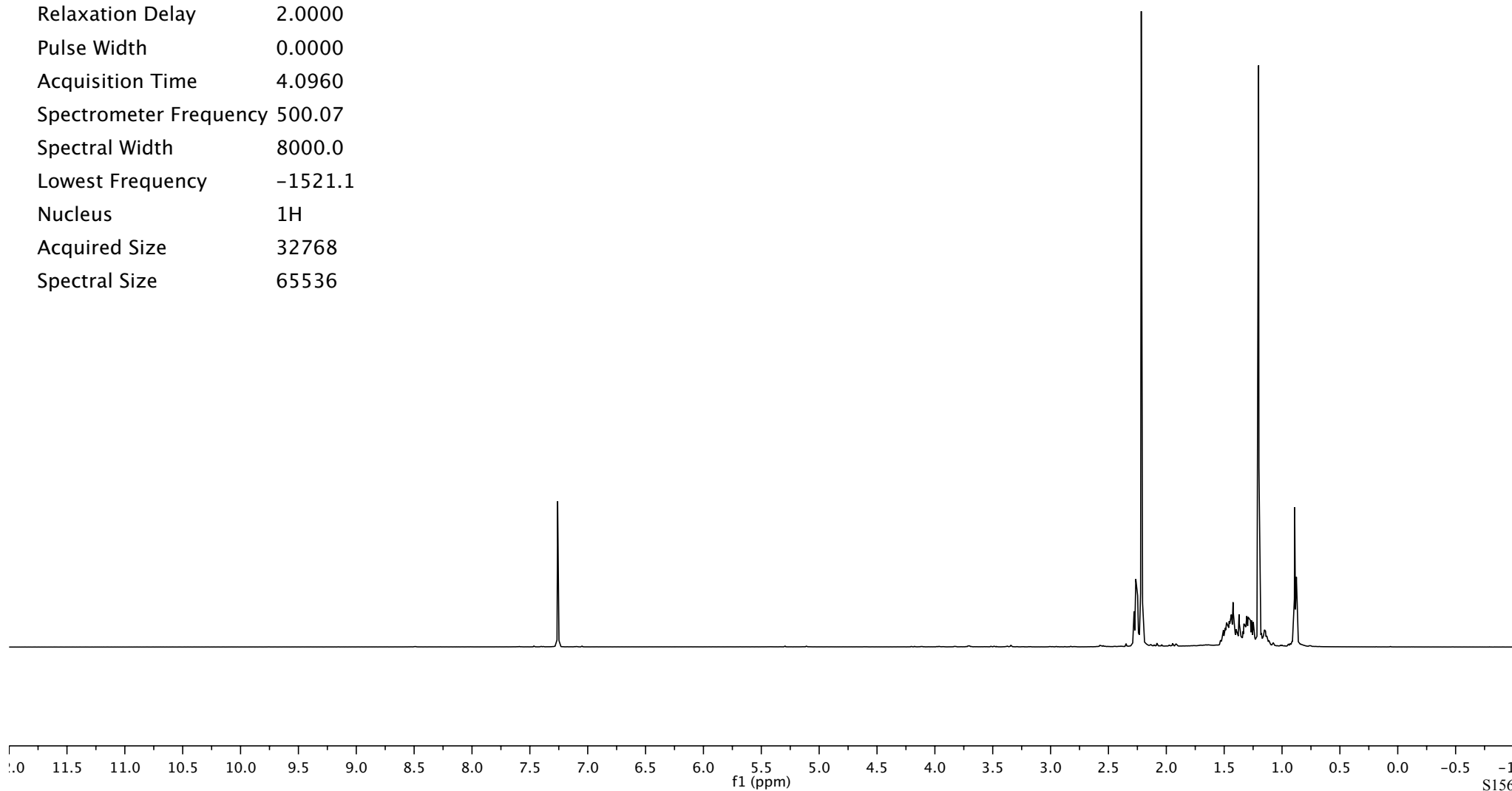
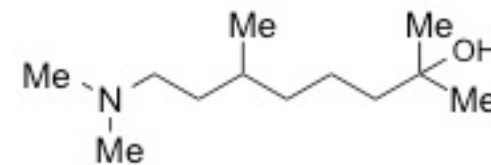
77.48 CDCl₃
77.16 CDCl₃
76.84 CDCl₃

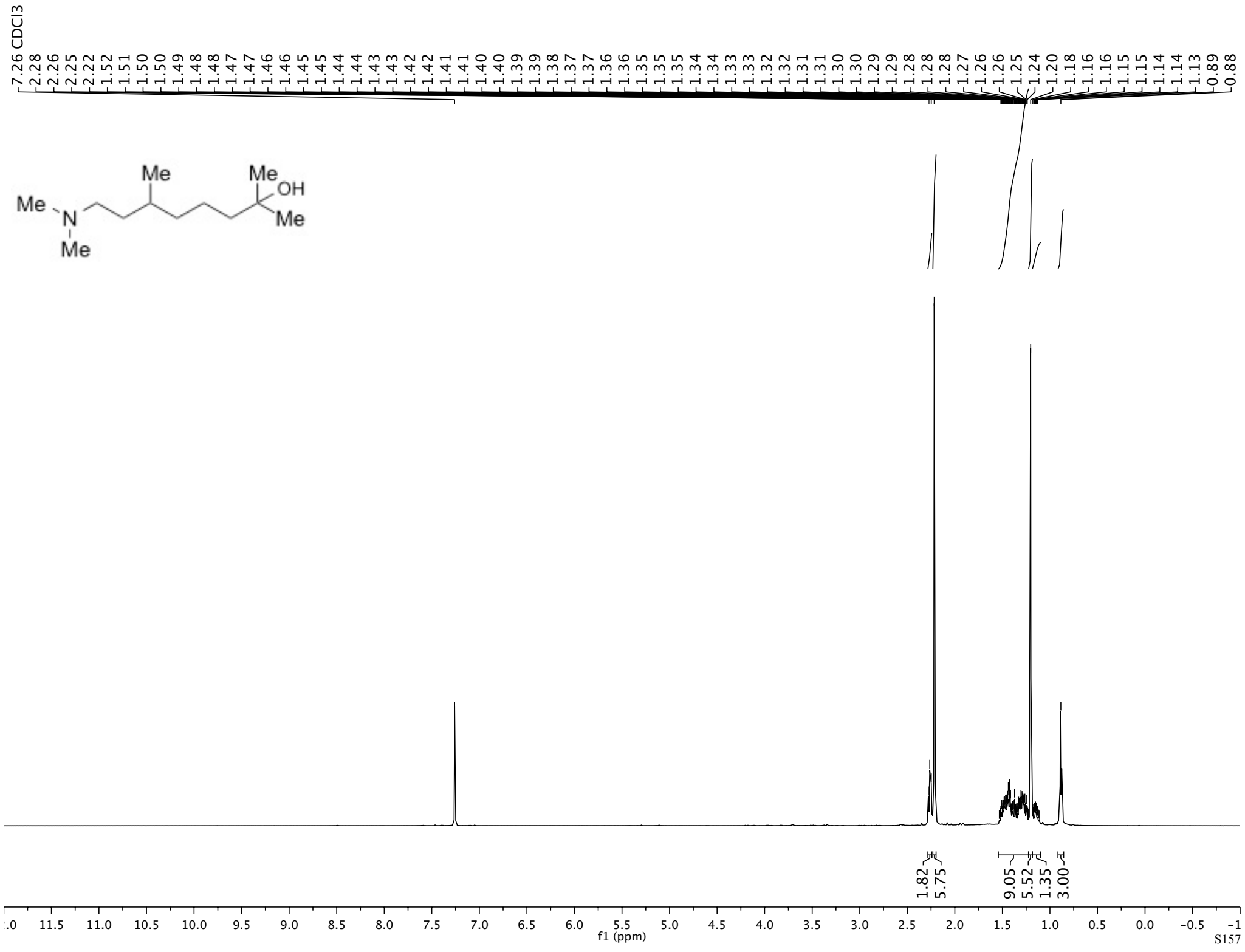
42.47
36.24
28.98

—7.84

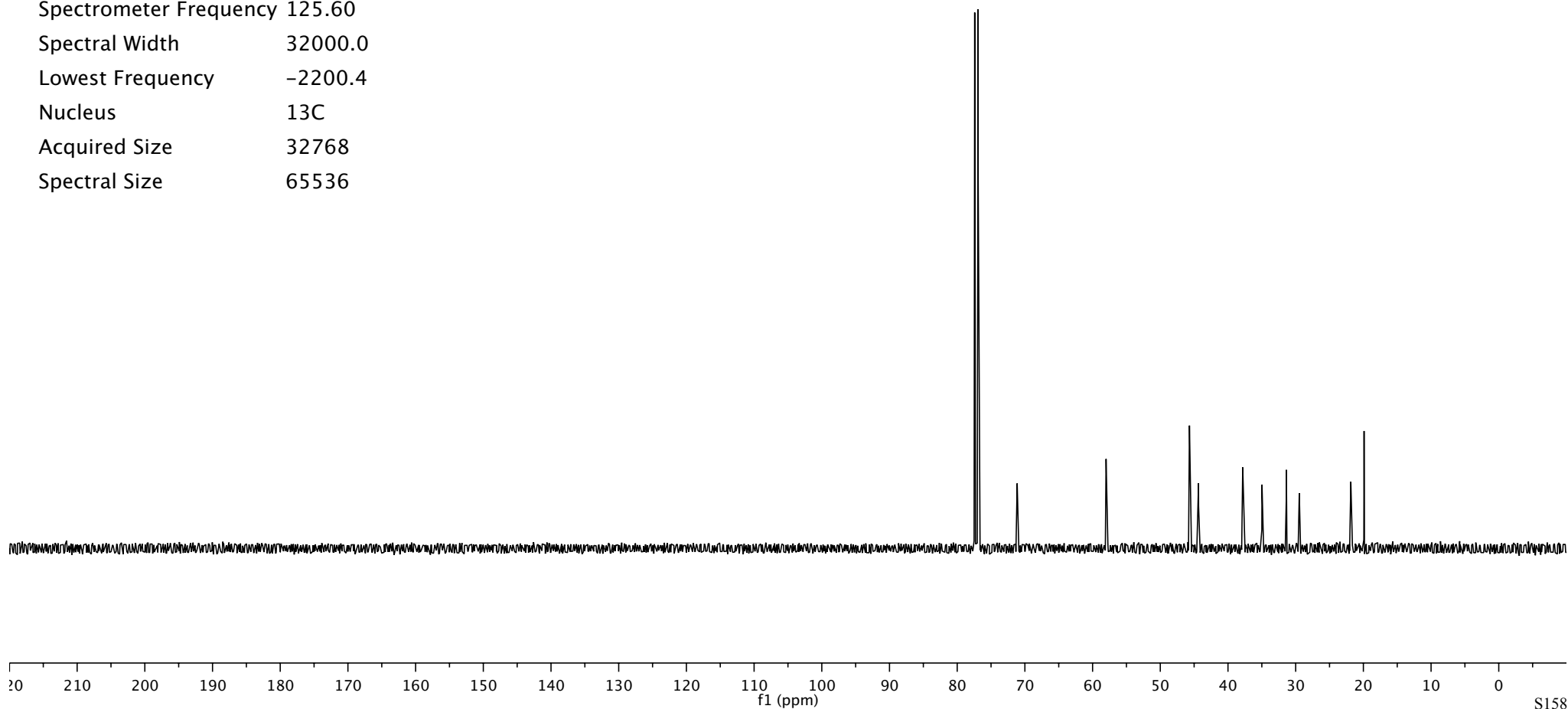
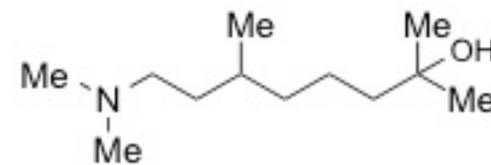


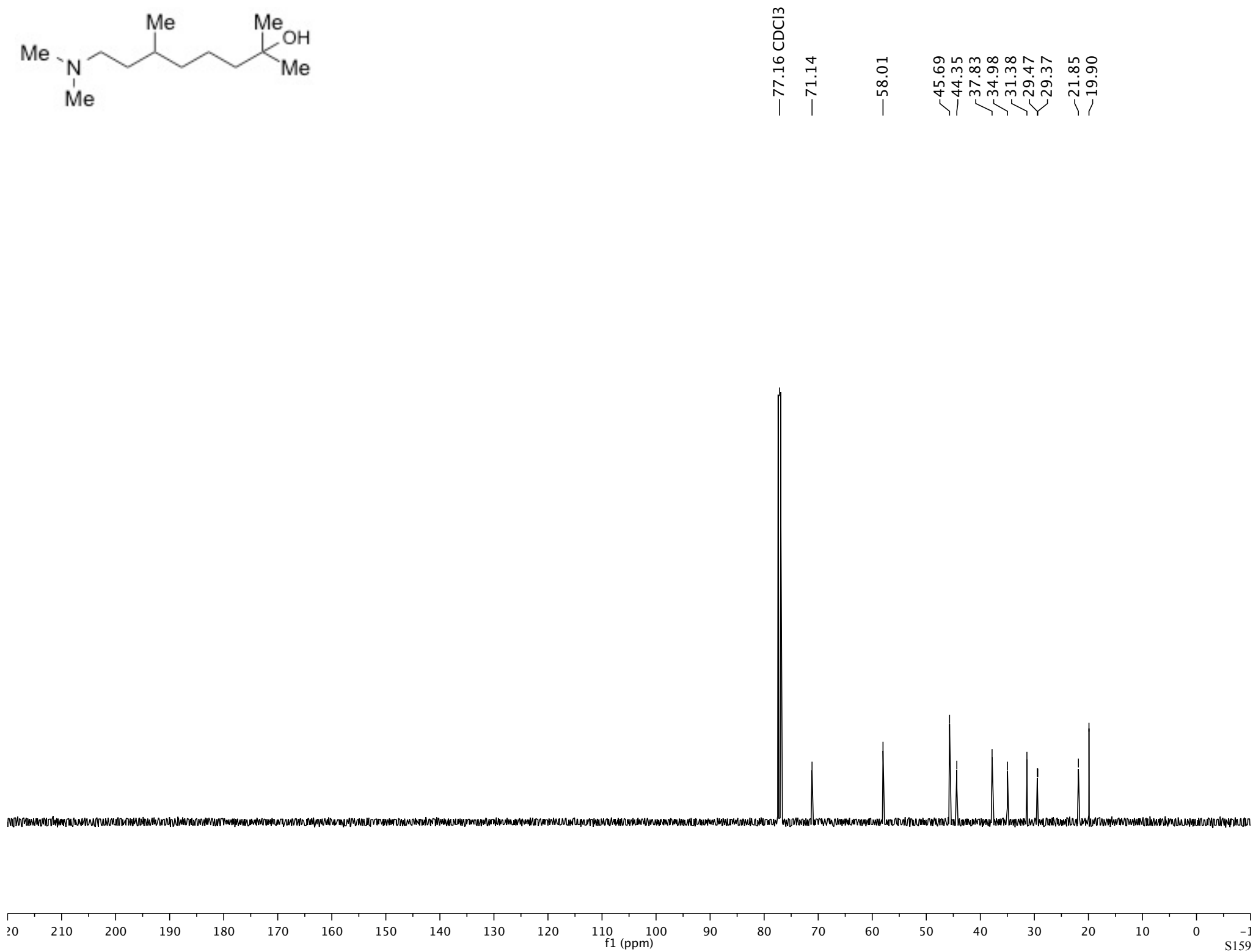
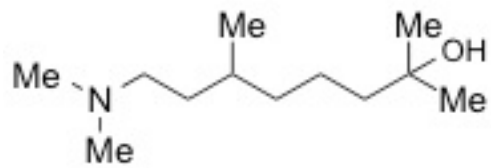
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	32
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



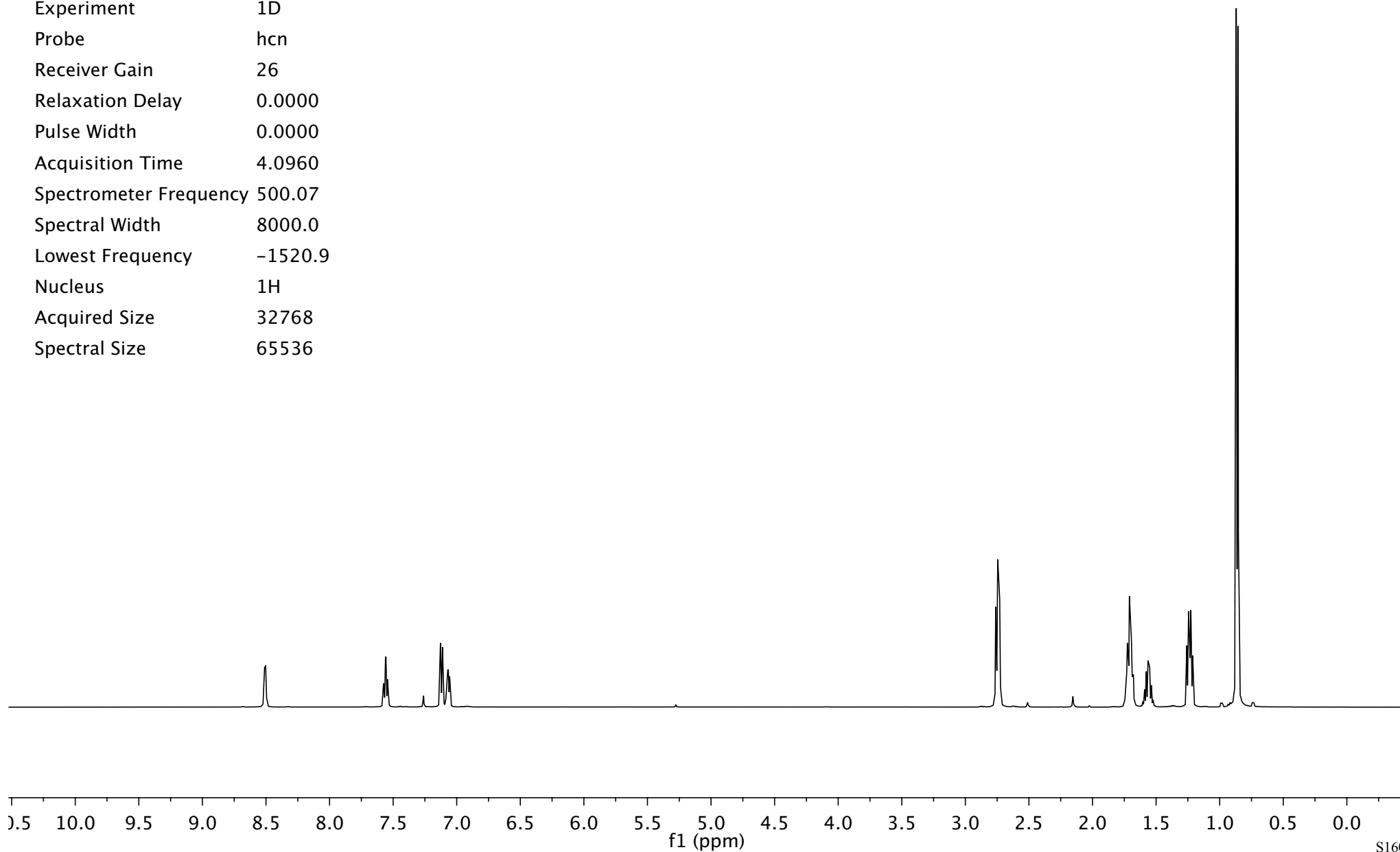
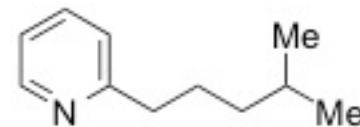


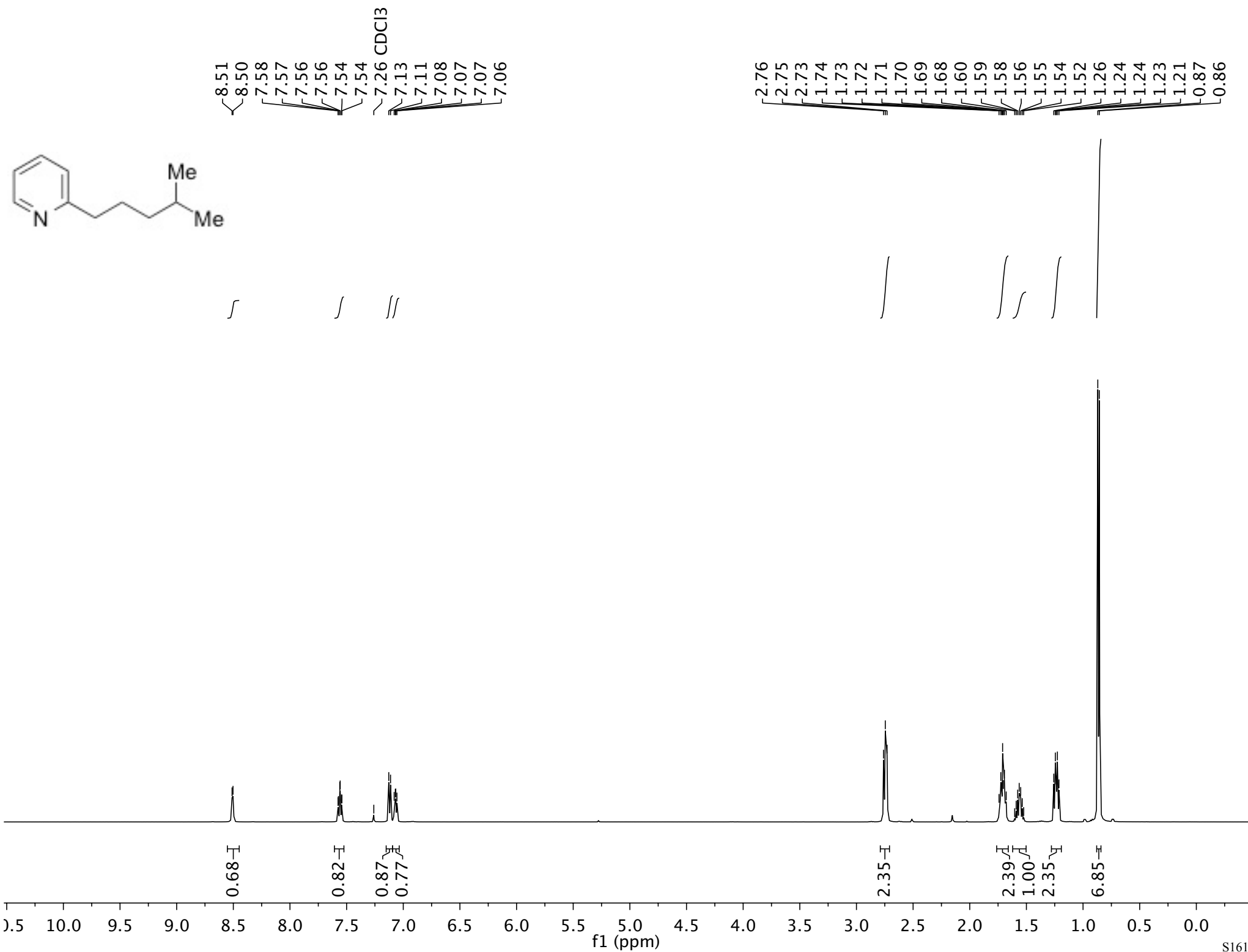
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Number of Scans	783
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2200.4
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



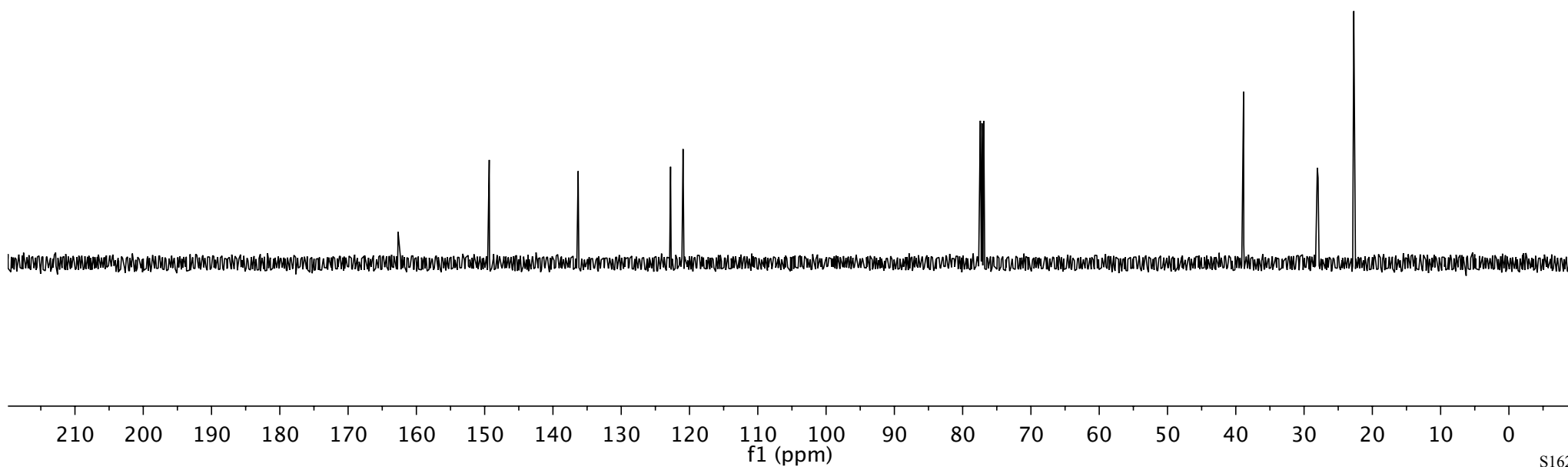
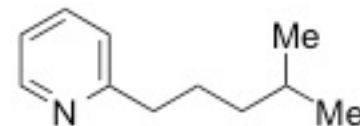


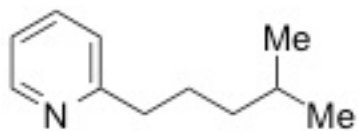
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	26
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1520.9
Nucleus	1H
Acquired Size	32768
Spectral Size	65536





Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2204.6
Nucleus	13C
Acquired Size	32768
Spectral Size	65536





—162.68

—149.33

—136.31

~122.77

~120.95

{77.42 CDCI3

{77.16 CDCI3

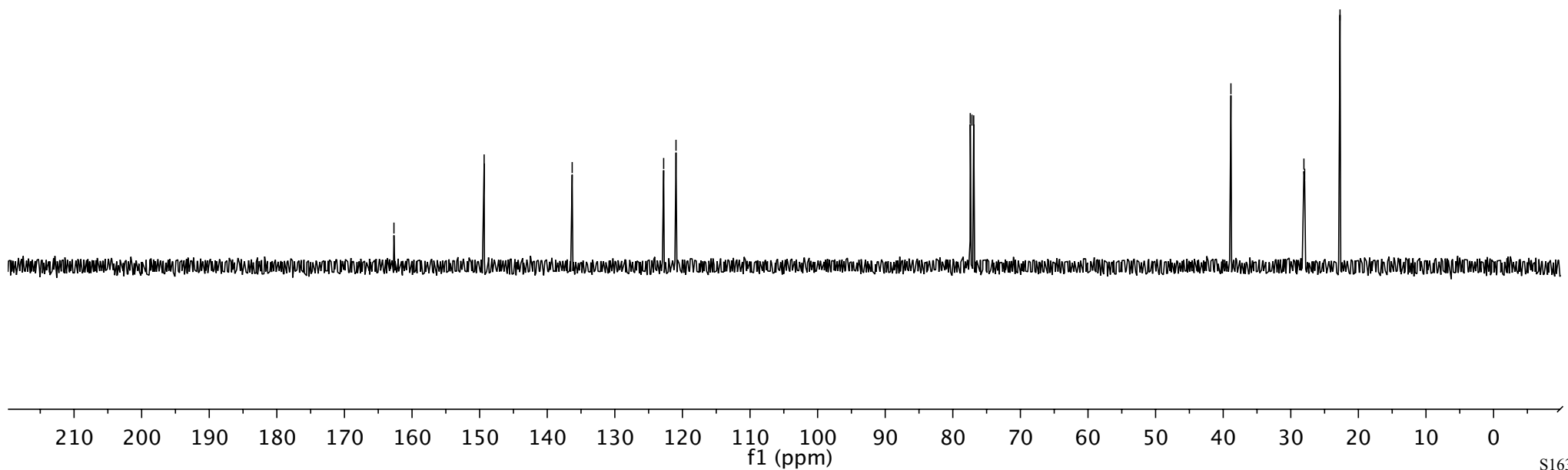
{76.91 CDCI3

—38.86

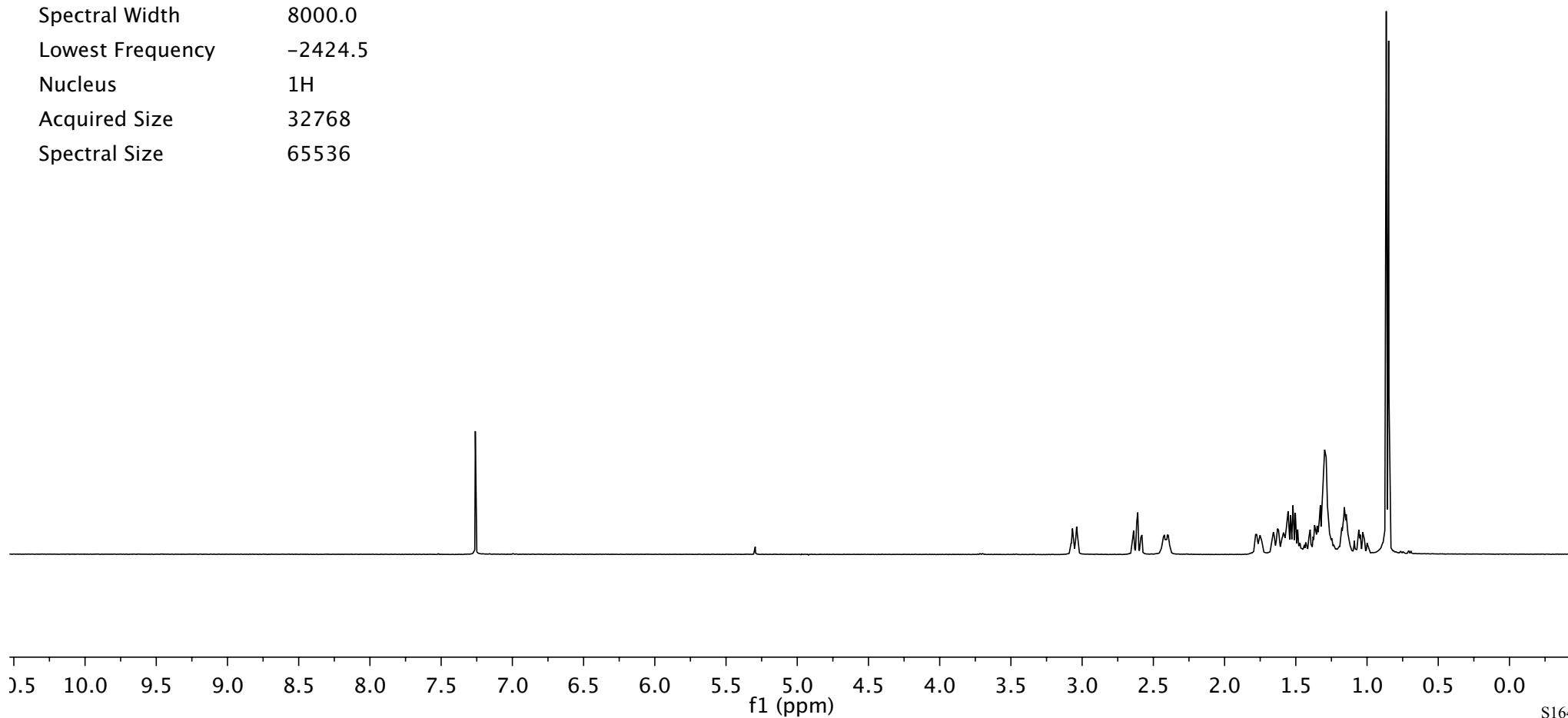
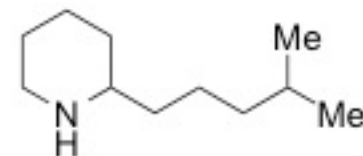
~28.06

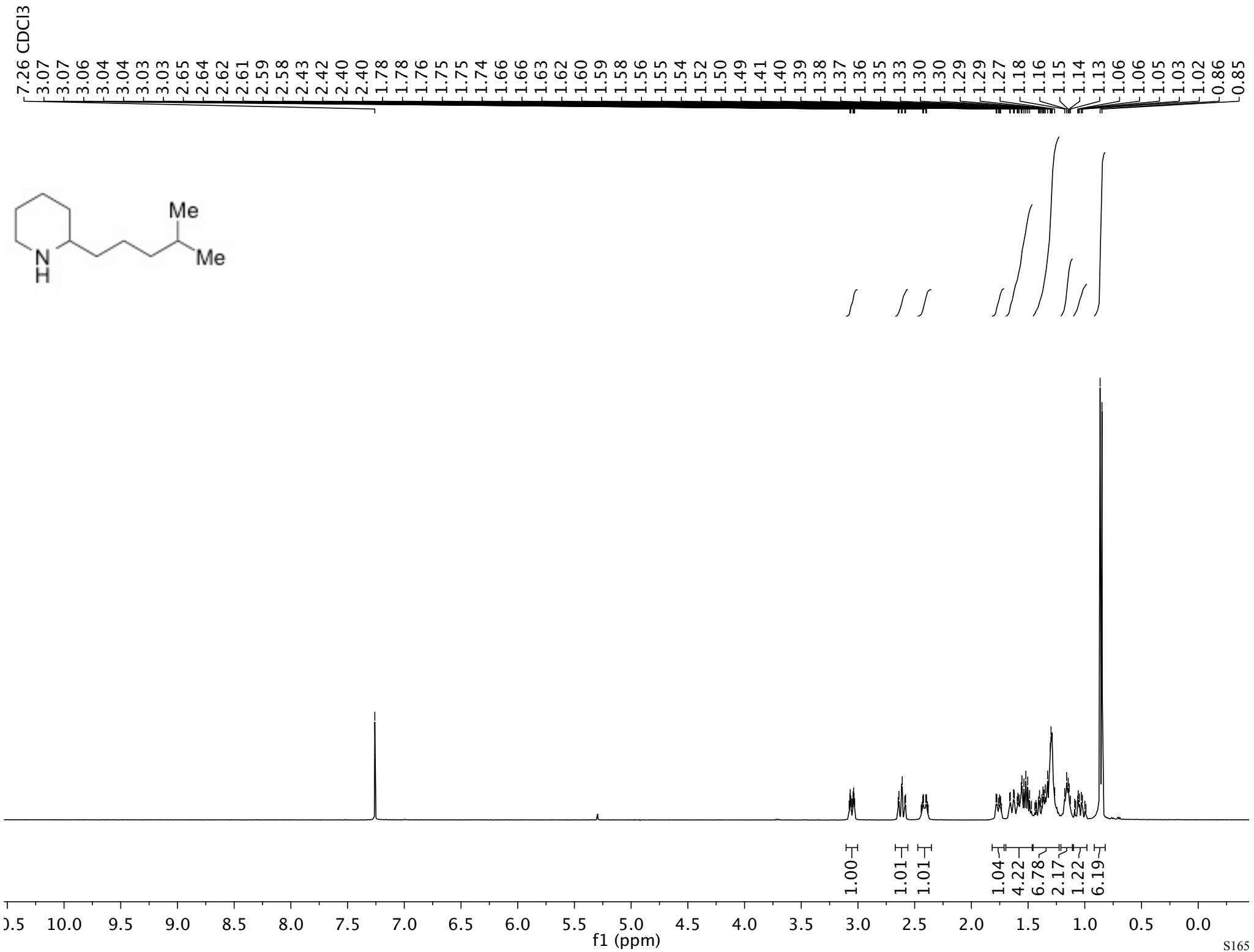
~27.95

~22.72

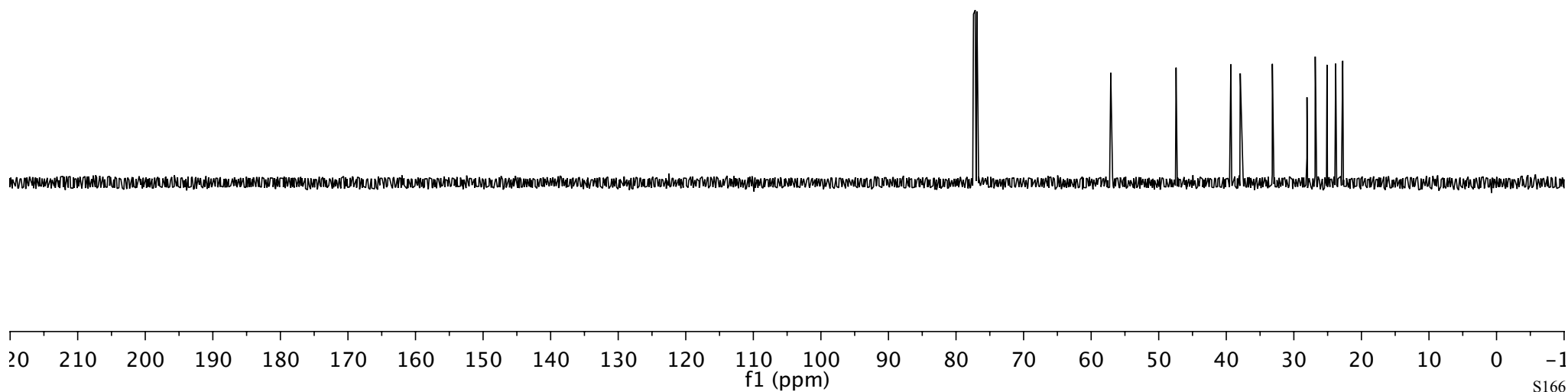
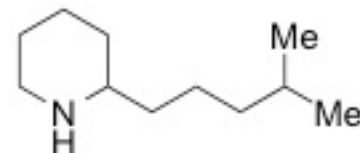


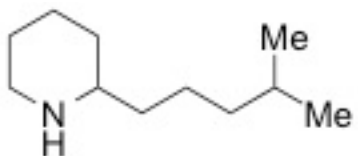
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	54
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	399.95
Spectral Width	8000.0
Lowest Frequency	-2424.5
Nucleus	1H
Acquired Size	32768
Spectral Size	65536





Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1272.5
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536





77.41 CDCl₃
 77.16 CDCl₃
 76.91 CDCl₃

—57.10

—47.43

39.32

37.93

33.18

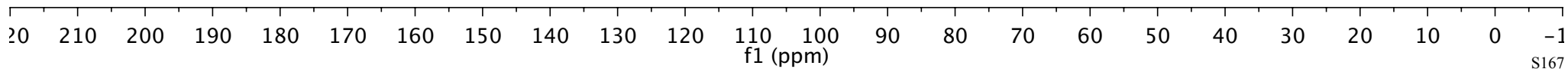
28.06

26.83

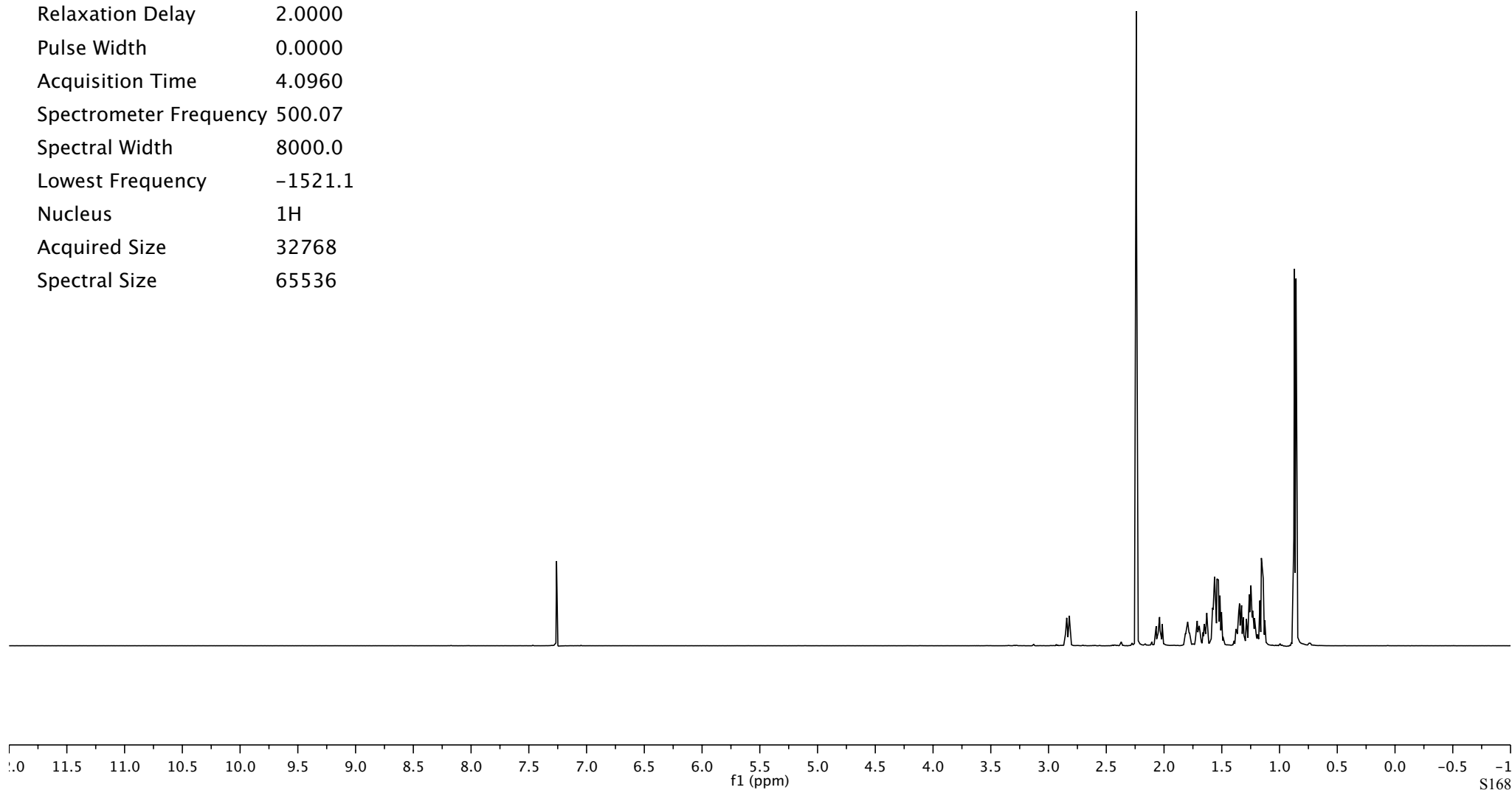
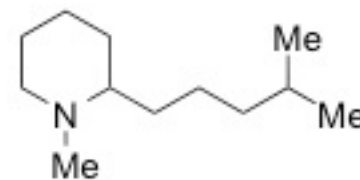
25.09

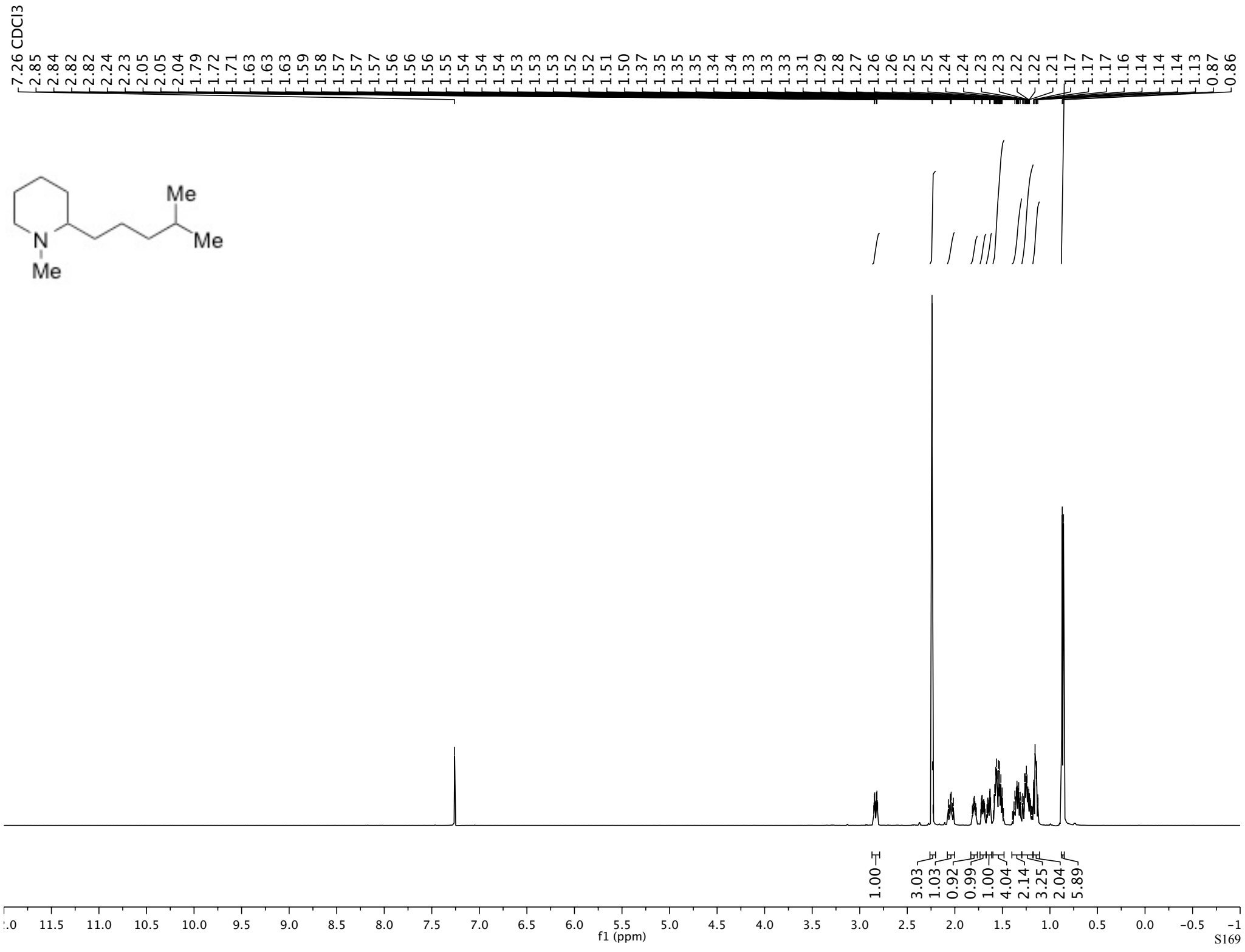
23.81

22.76

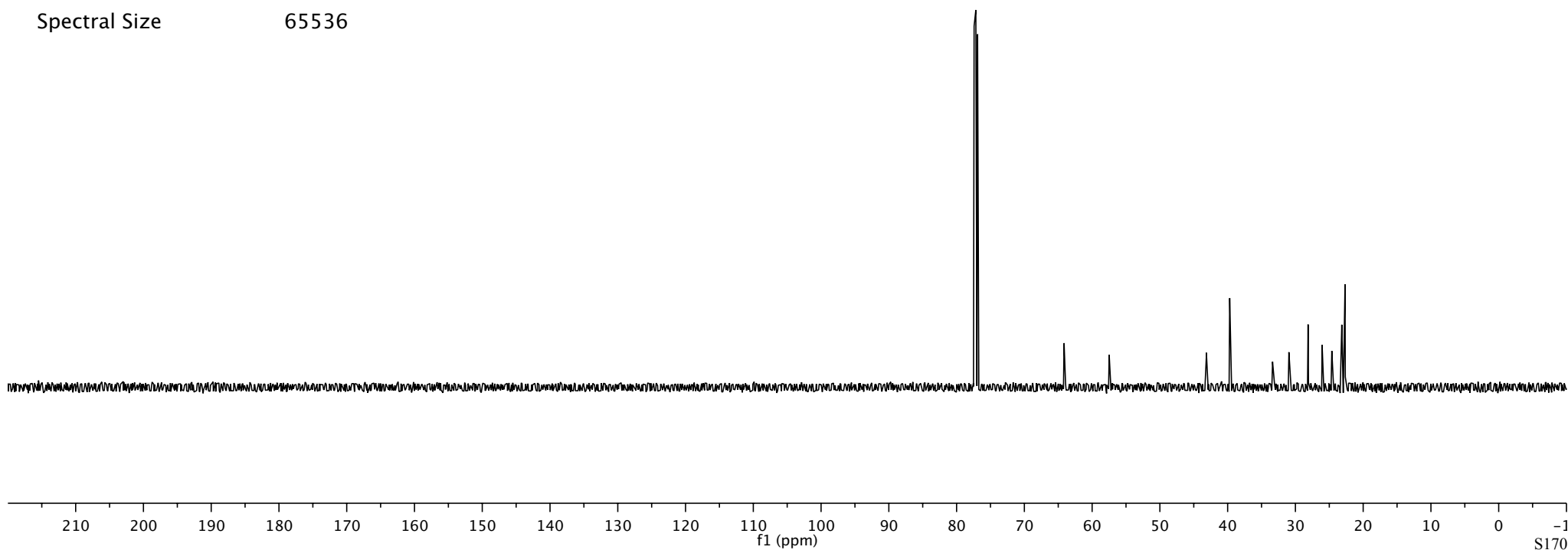
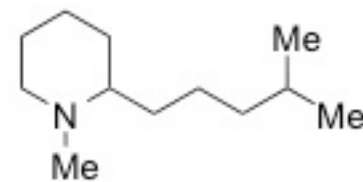


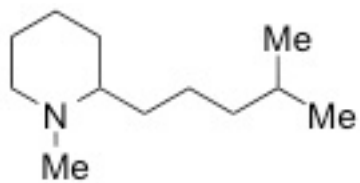
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	32
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536





Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Number of Scans	704
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2199.8
Nucleus	13C
Acquired Size	32768
Spectral Size	65536





—77.16 CDCl₃

—64.14

—57.48

43.14

39.69

33.37

30.96

28.13

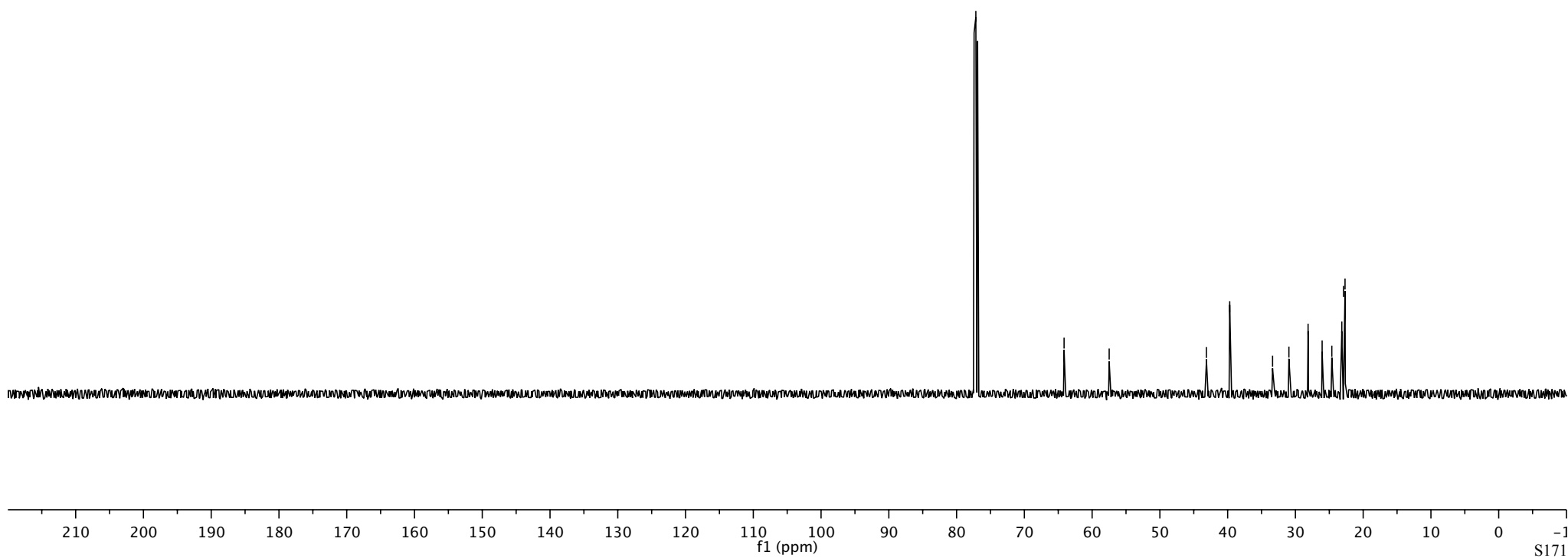
26.06

24.63

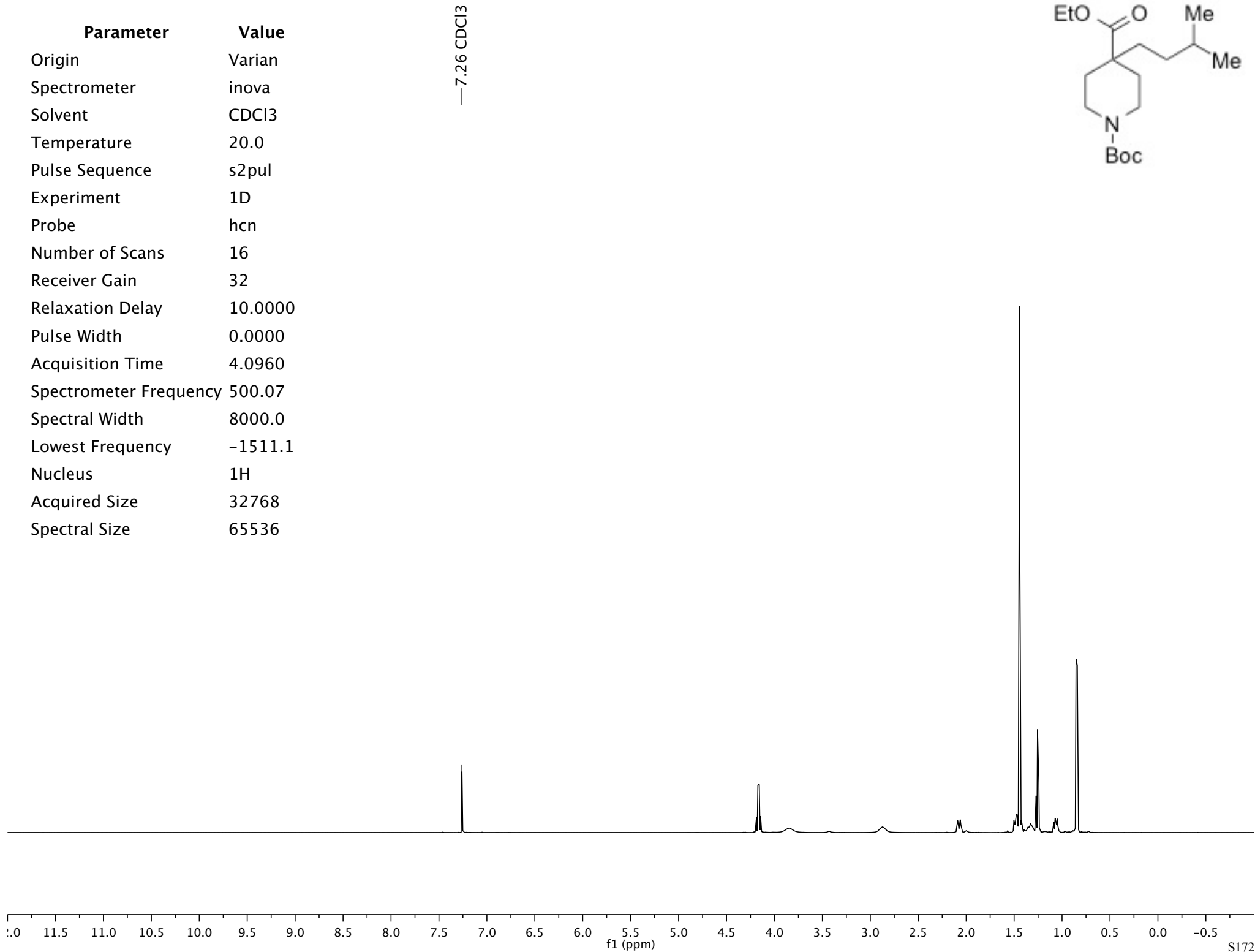
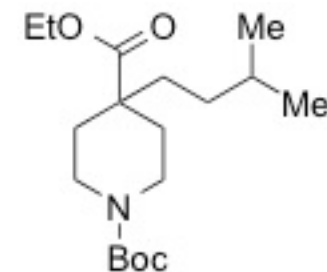
23.15

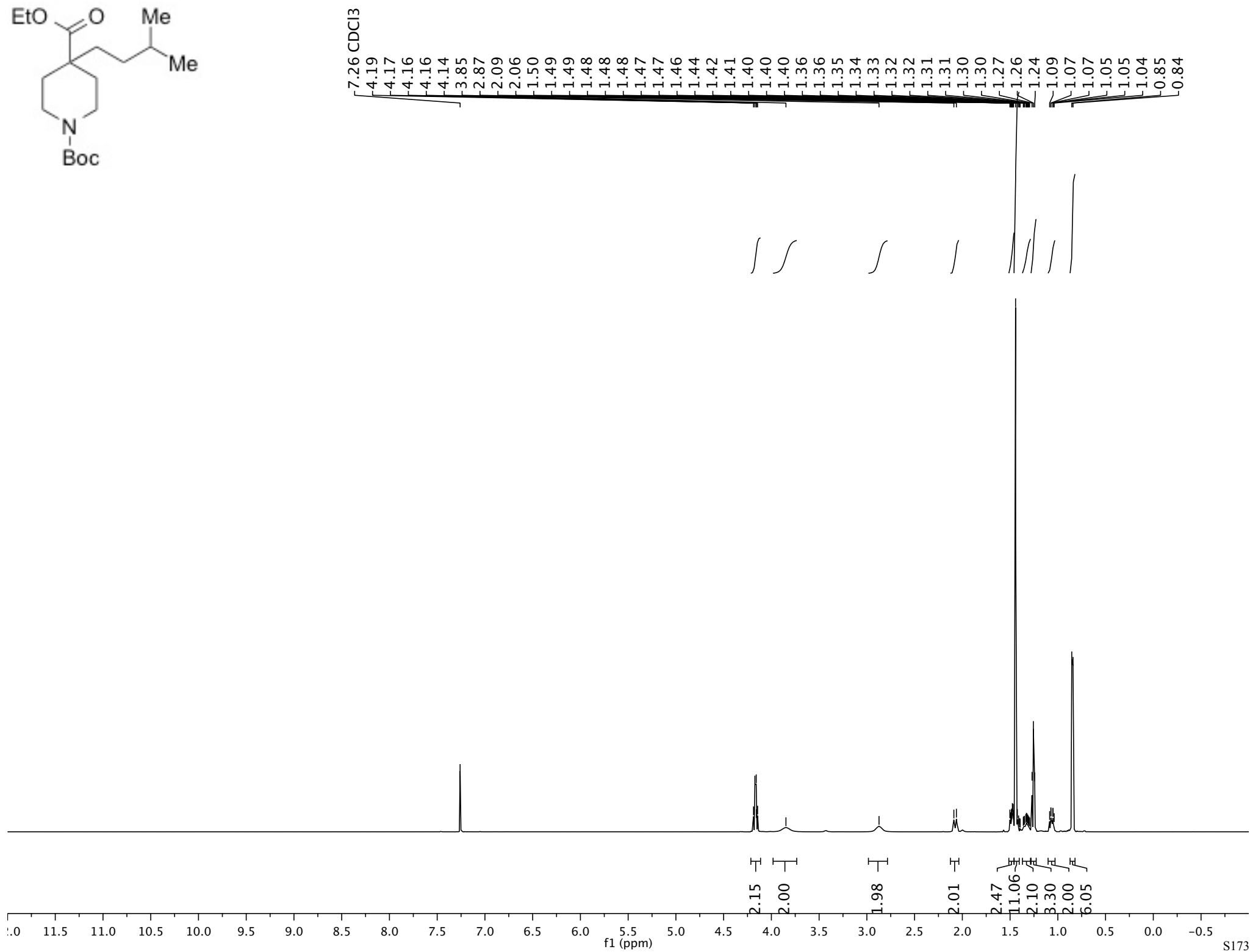
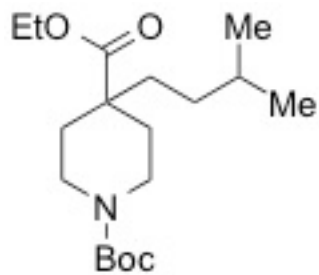
22.91

22.68

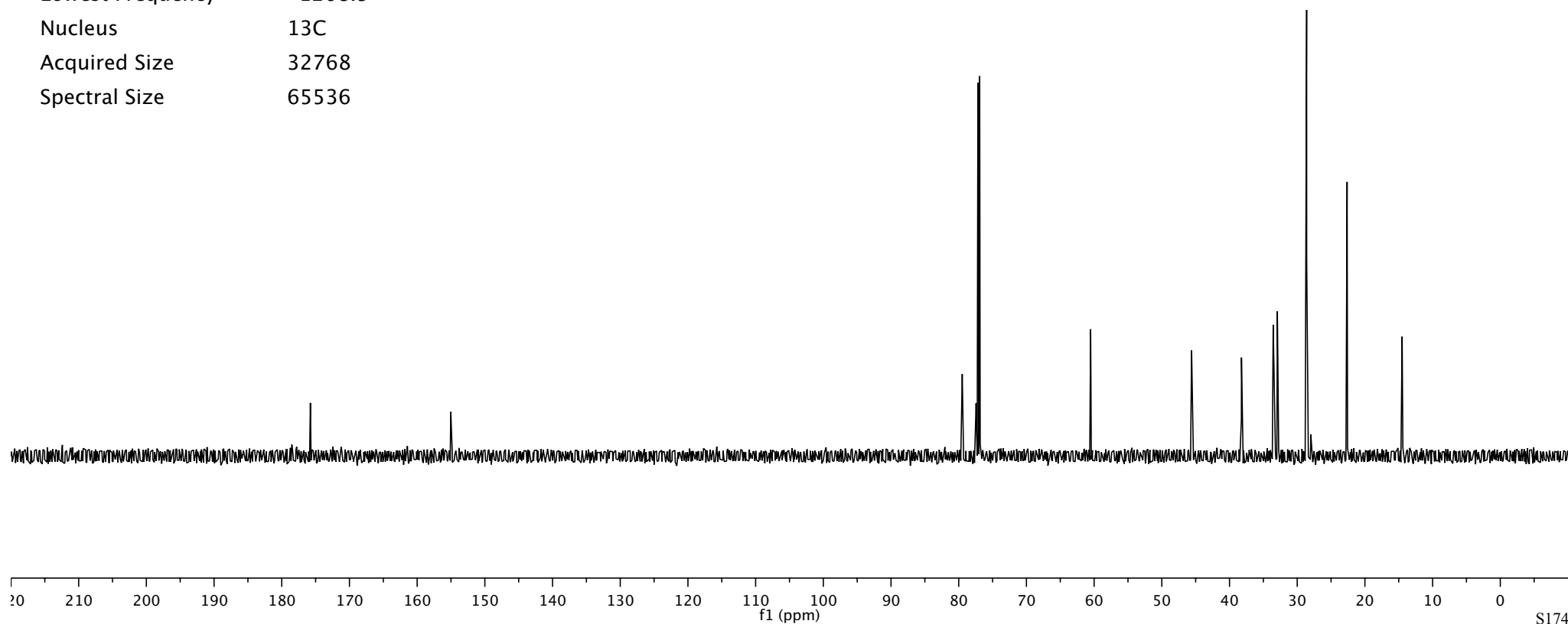
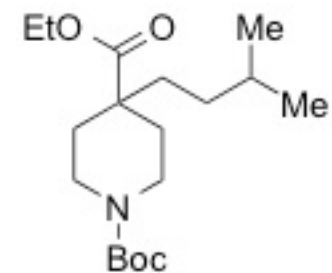


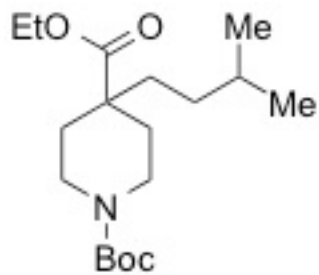
— 7.26 CDCl₃





Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	35.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	296
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1268.5
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536





—175.77

—155.03

~79.48
~77.16 CDCl₃

—60.51

—45.60

~38.23

~33.54

~32.93

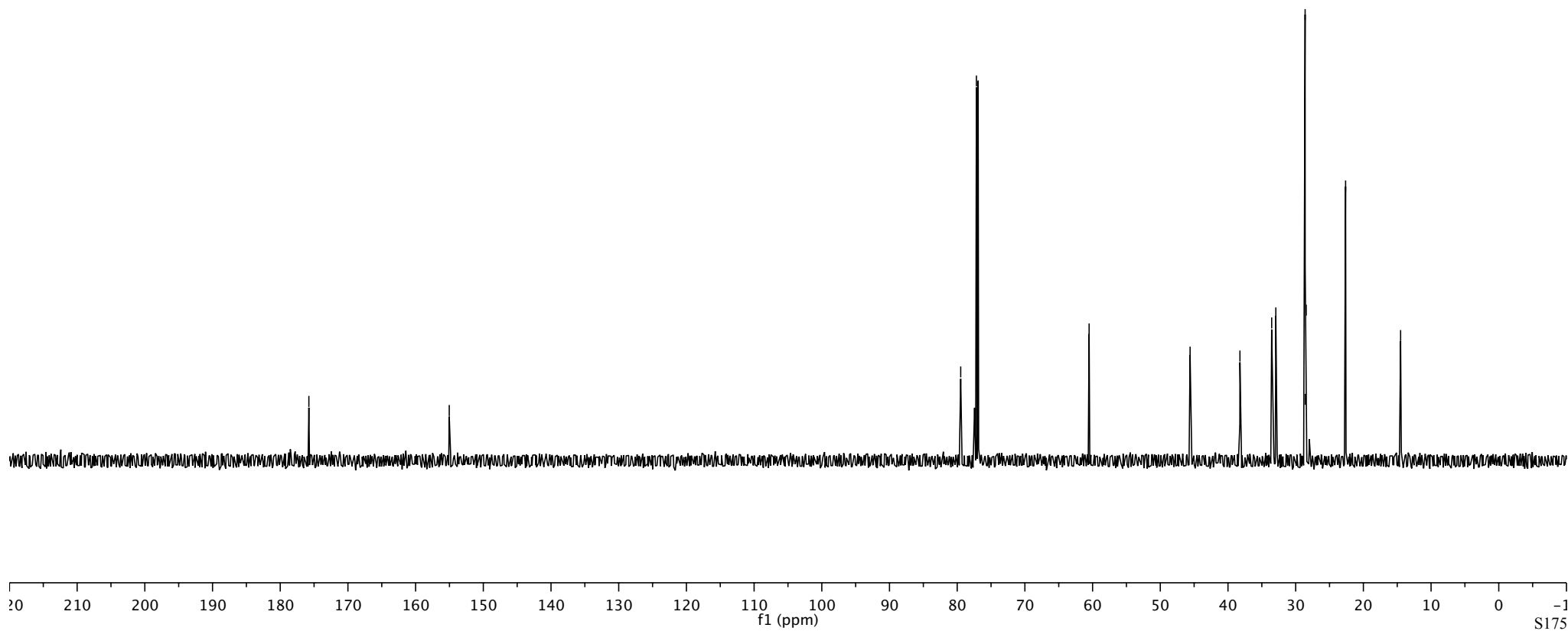
~28.60

~28.57

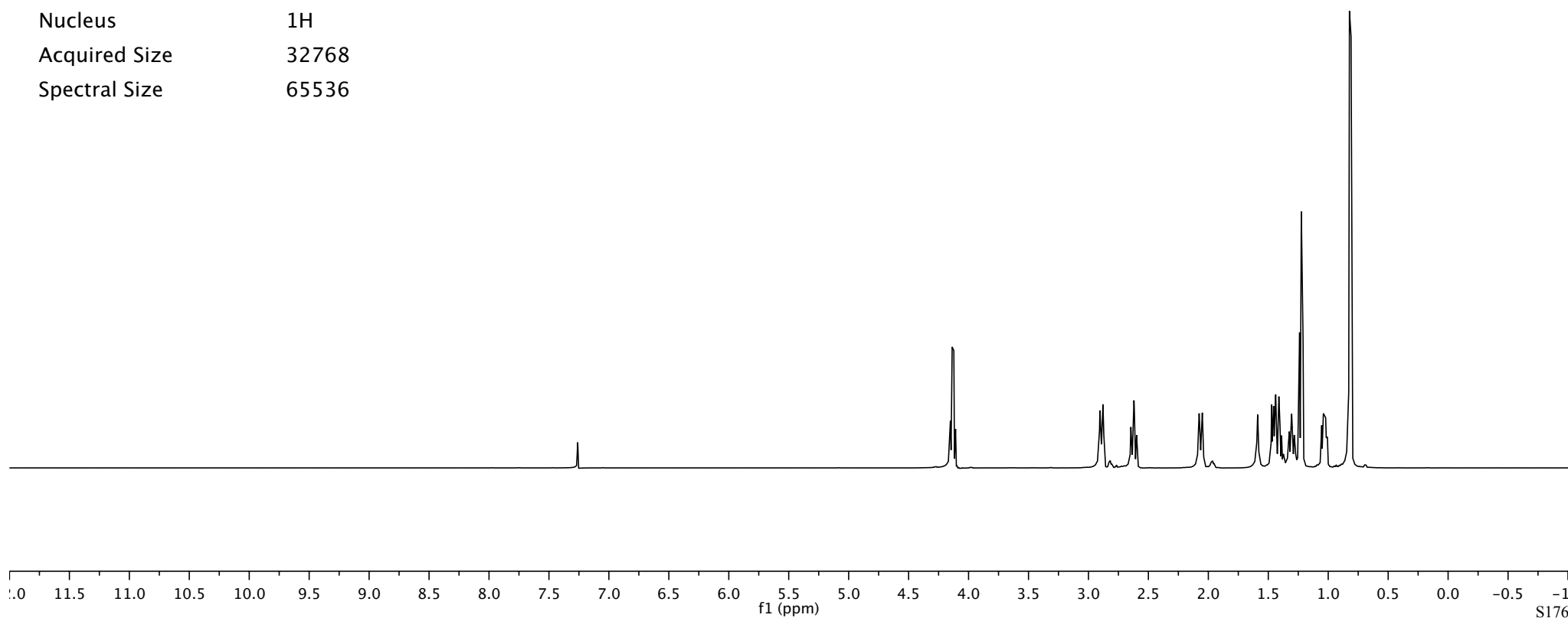
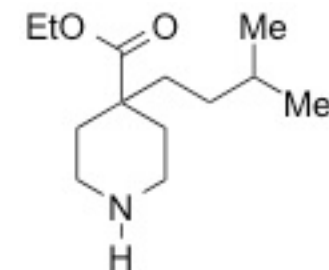
~28.45

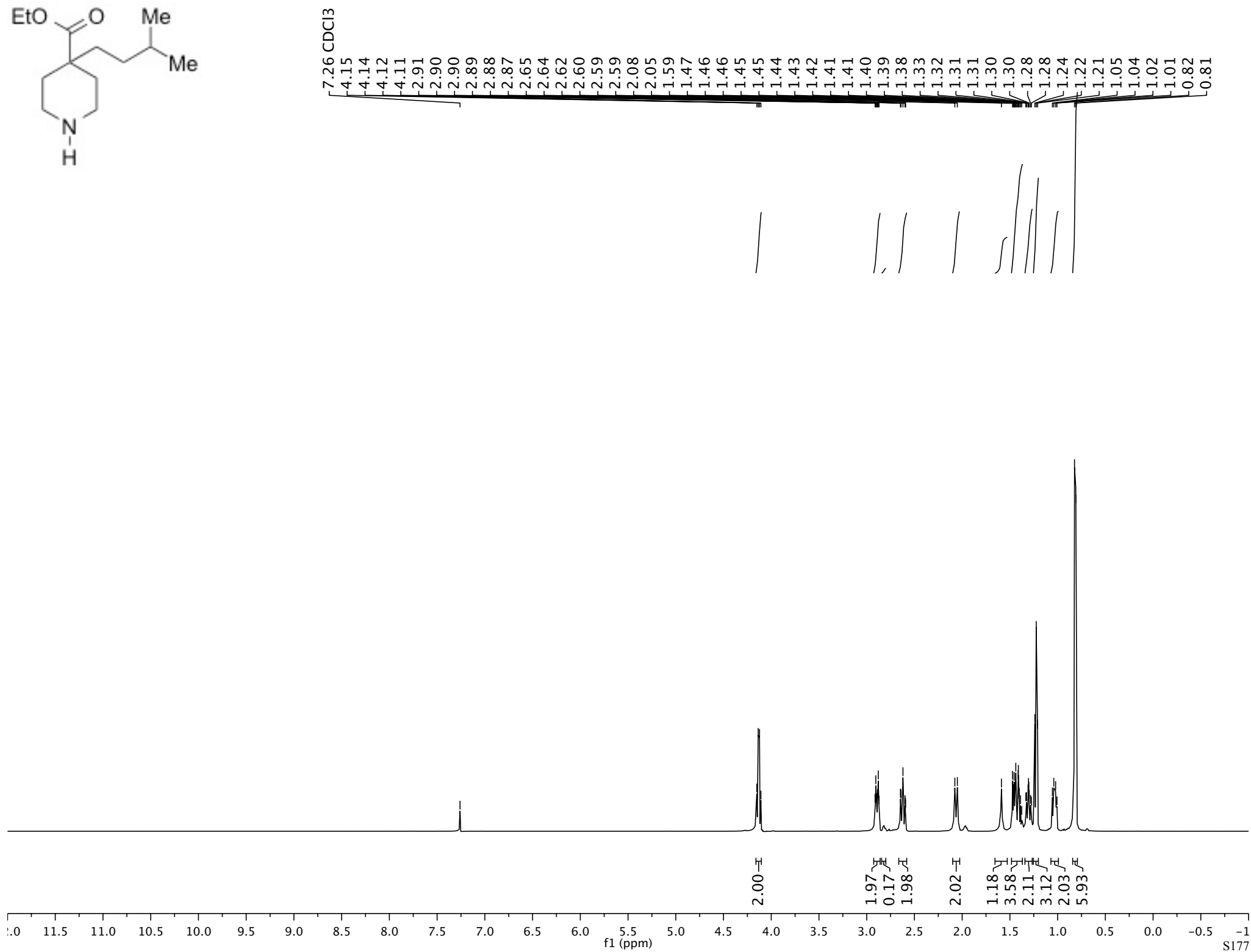
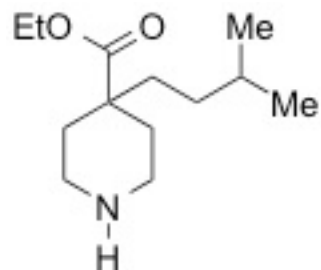
~22.63

—14.50

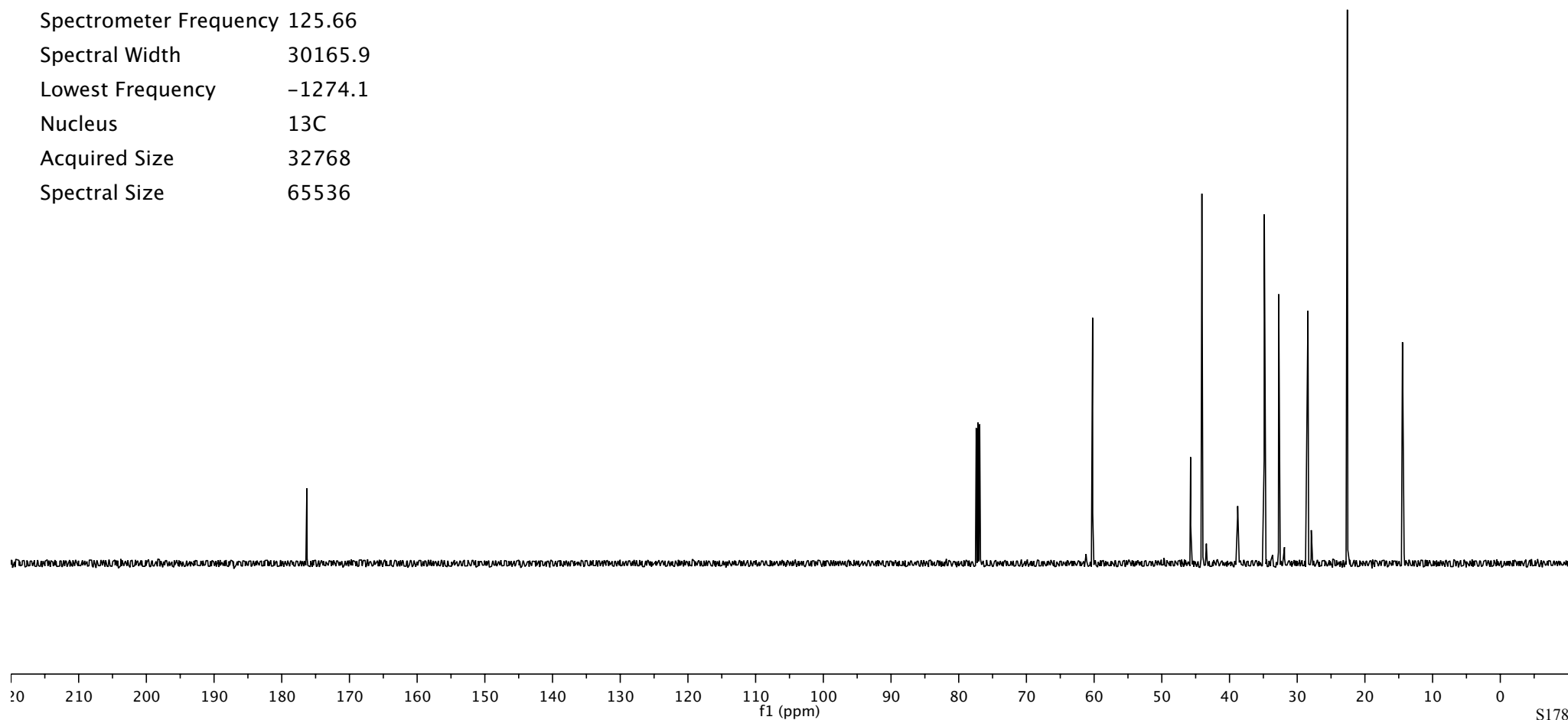
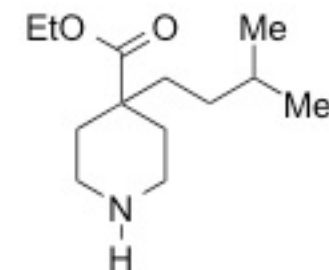


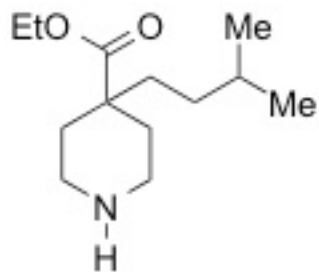
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	21.1
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	20
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1510.6
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536





Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	241
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1274.1
Nucleus	13C
Acquired Size	32768
Spectral Size	65536





—176.29

—77.16 CDCl₃

—60.22

—45.75

—44.08

—38.79

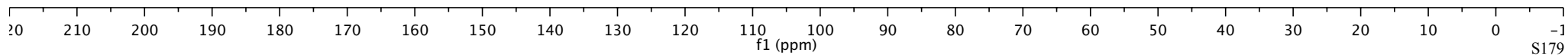
—34.86

—32.73

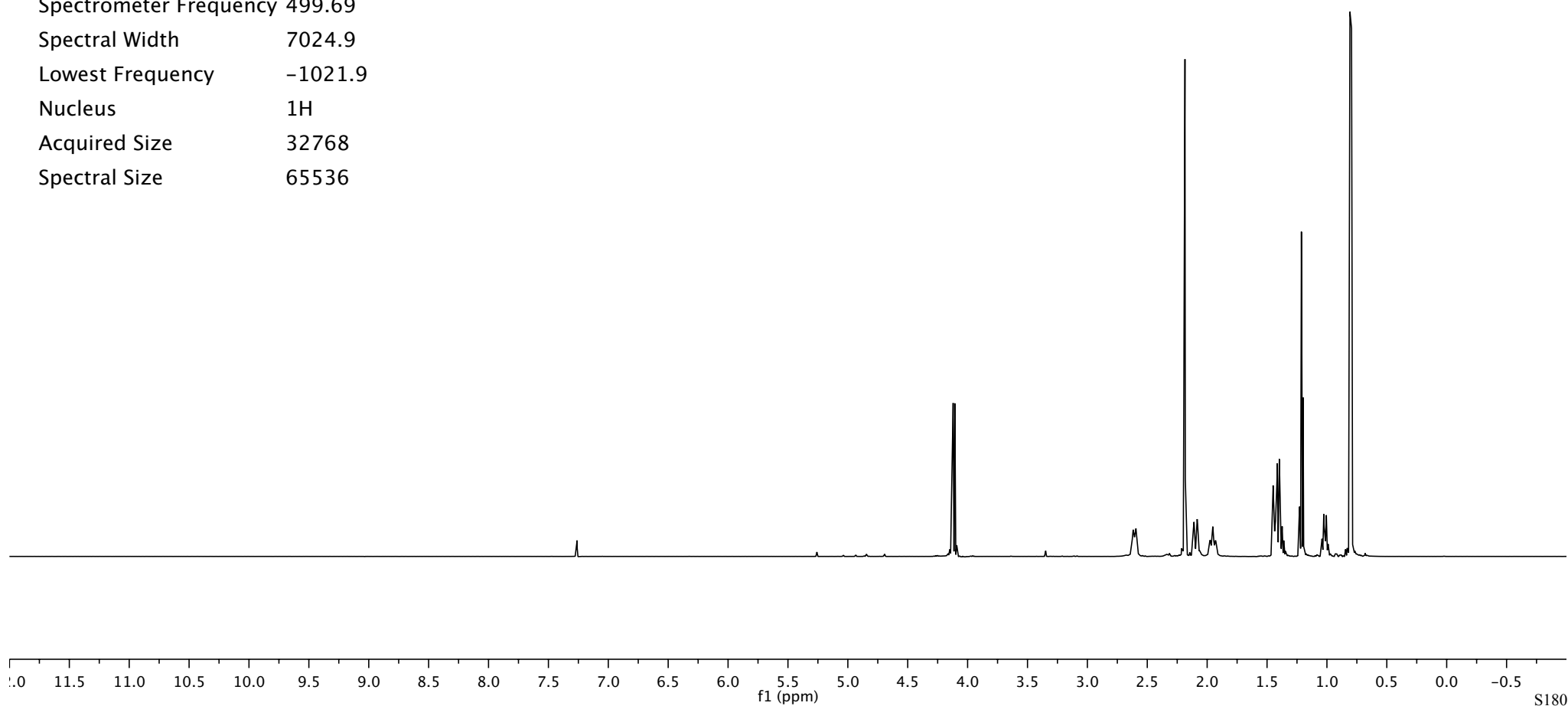
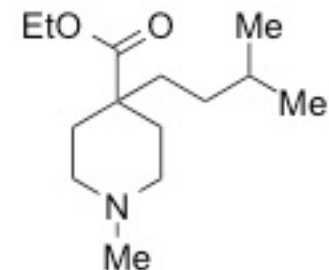
—28.41

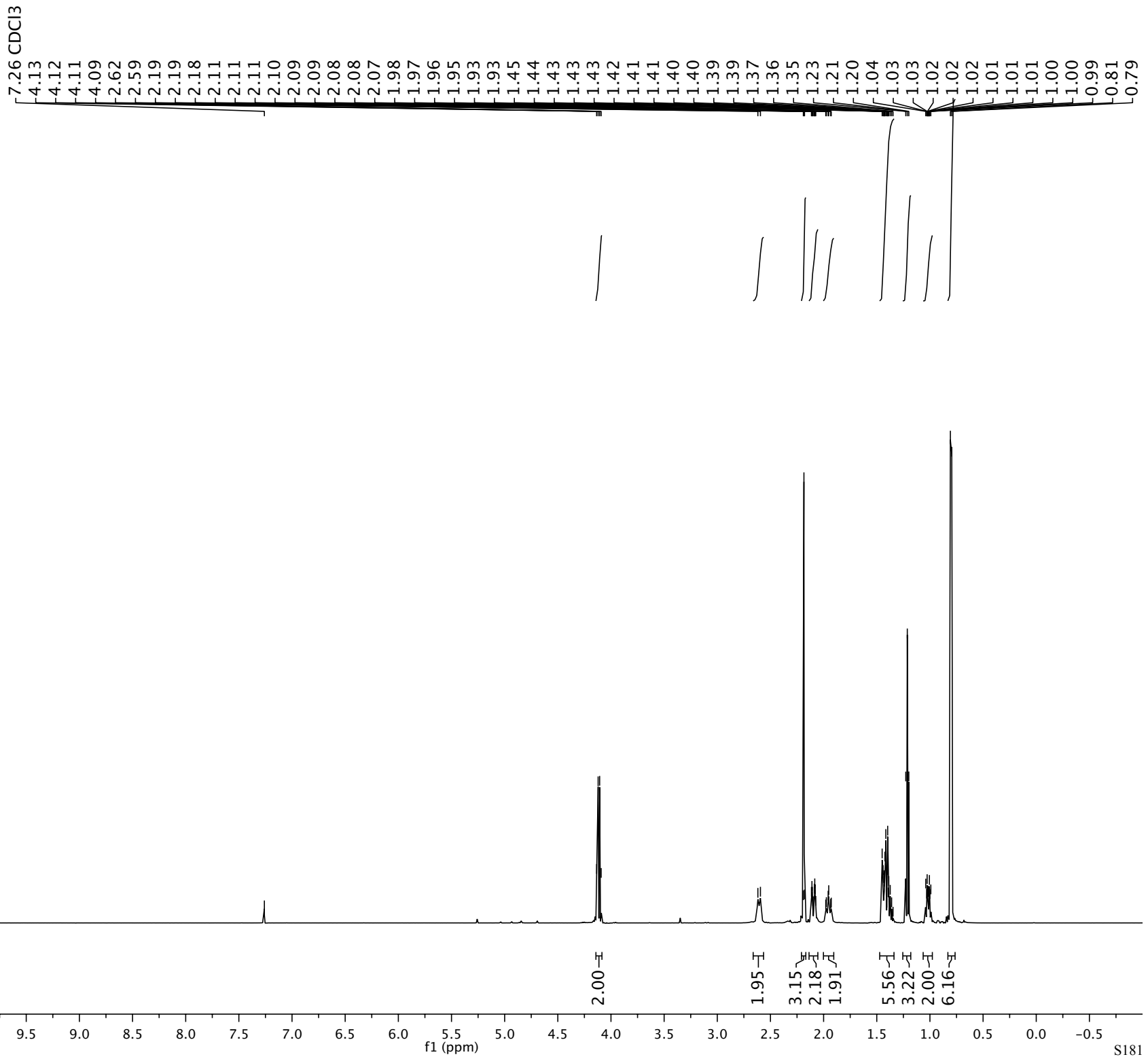
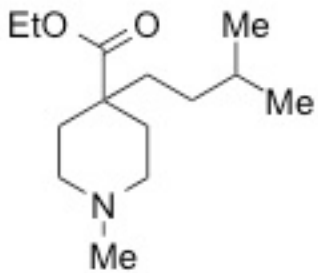
—22.59

—14.45

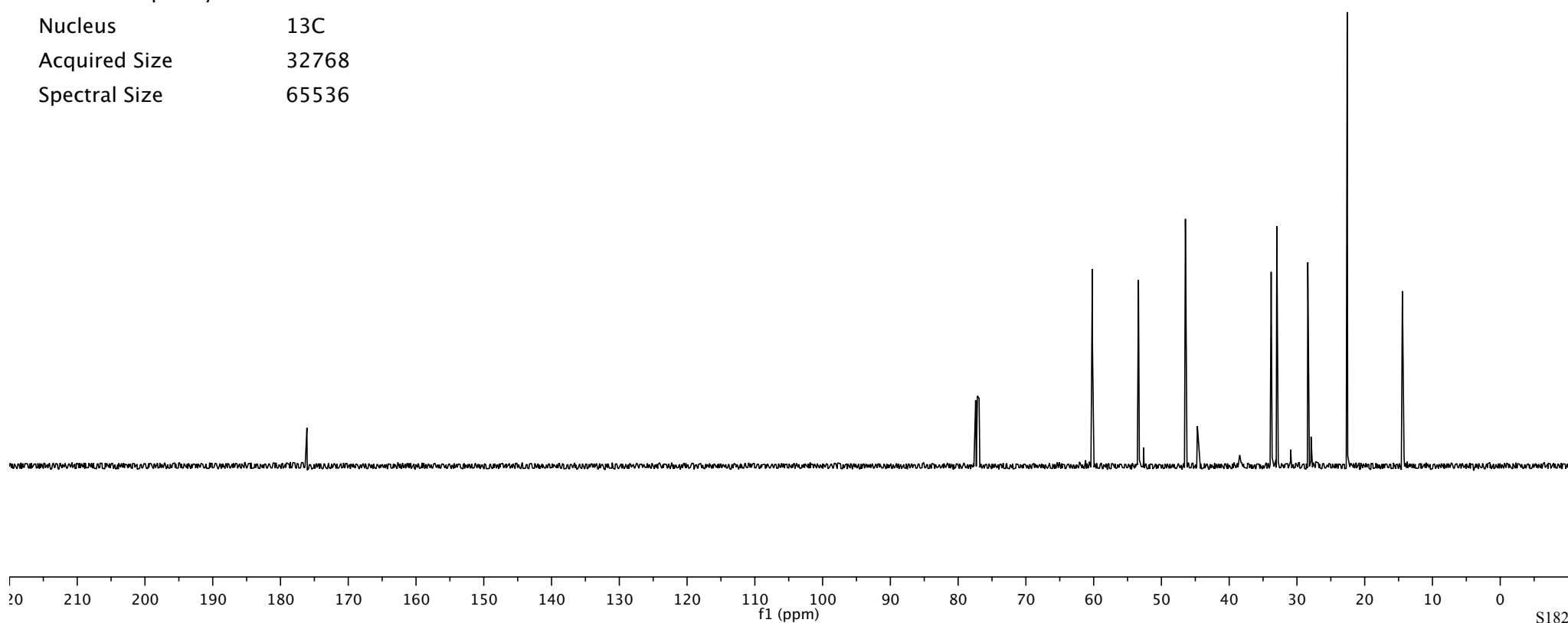
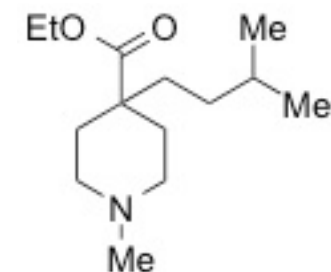


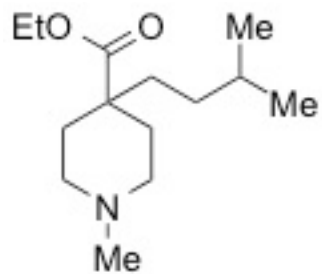
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	8
Receiver Gain	30
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.69
Spectral Width	7024.9
Lowest Frequency	-1021.9
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536





Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	80
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1276.3
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536





—176.10

—77.16 CDCl₃

—60.19

—53.39

—46.46

—44.69

—38.44

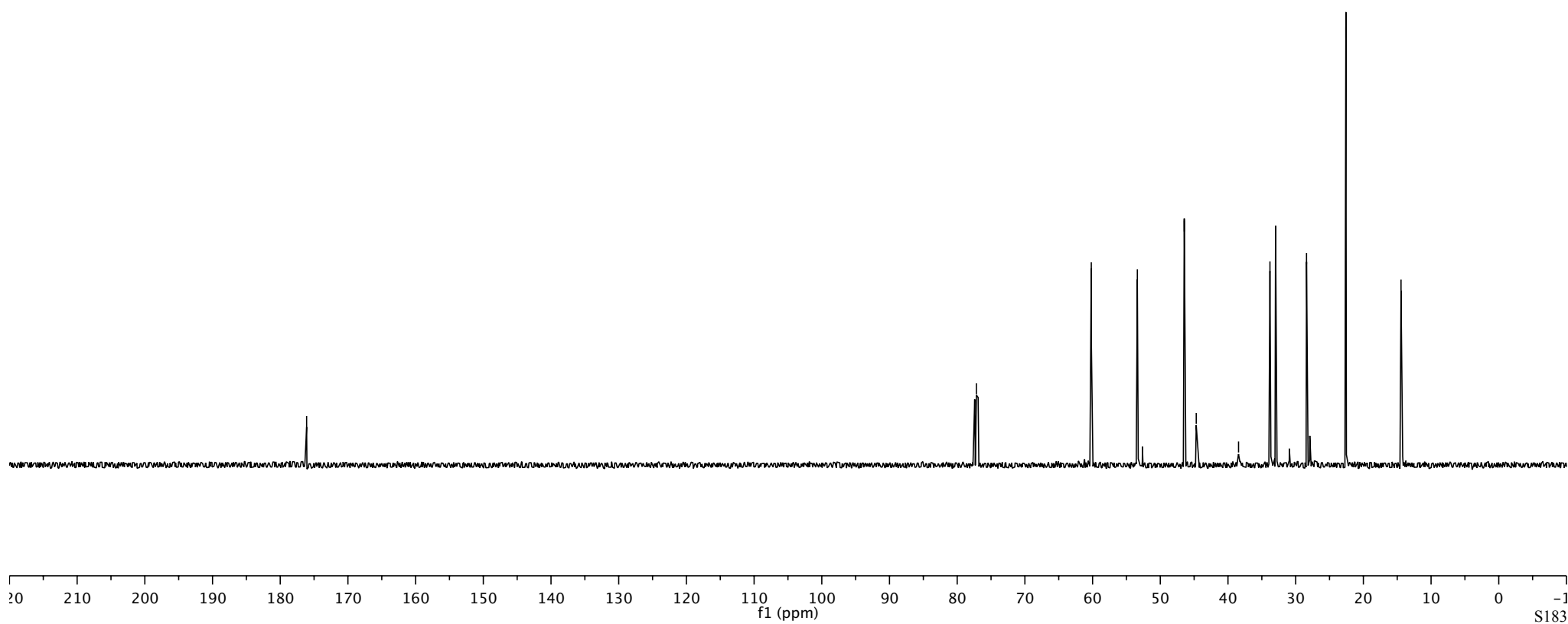
—33.80

—32.97

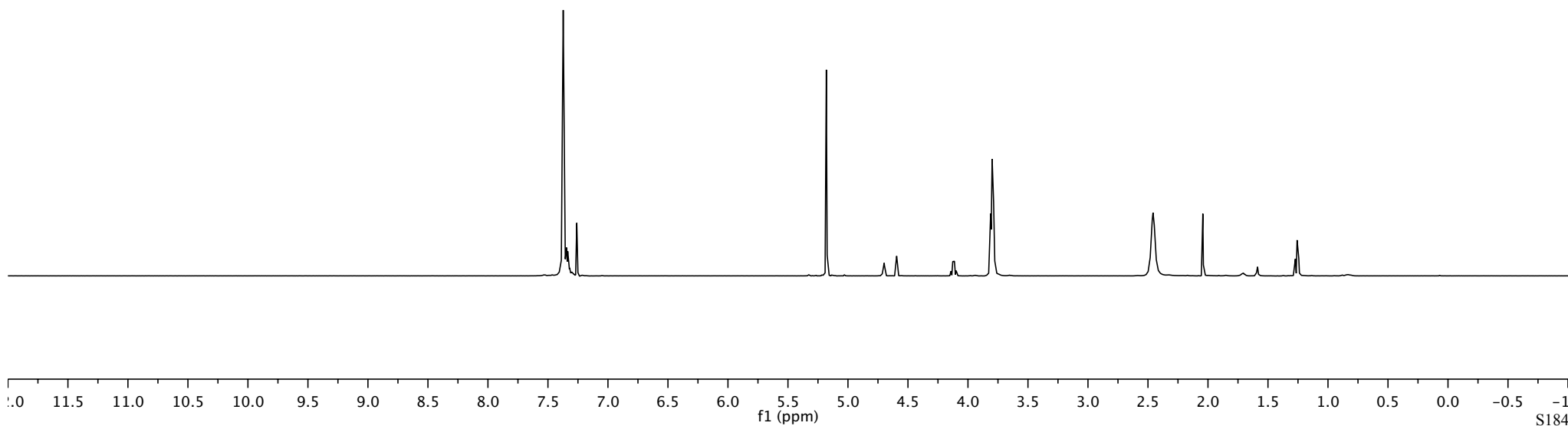
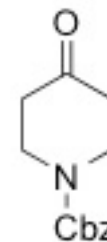
—28.40

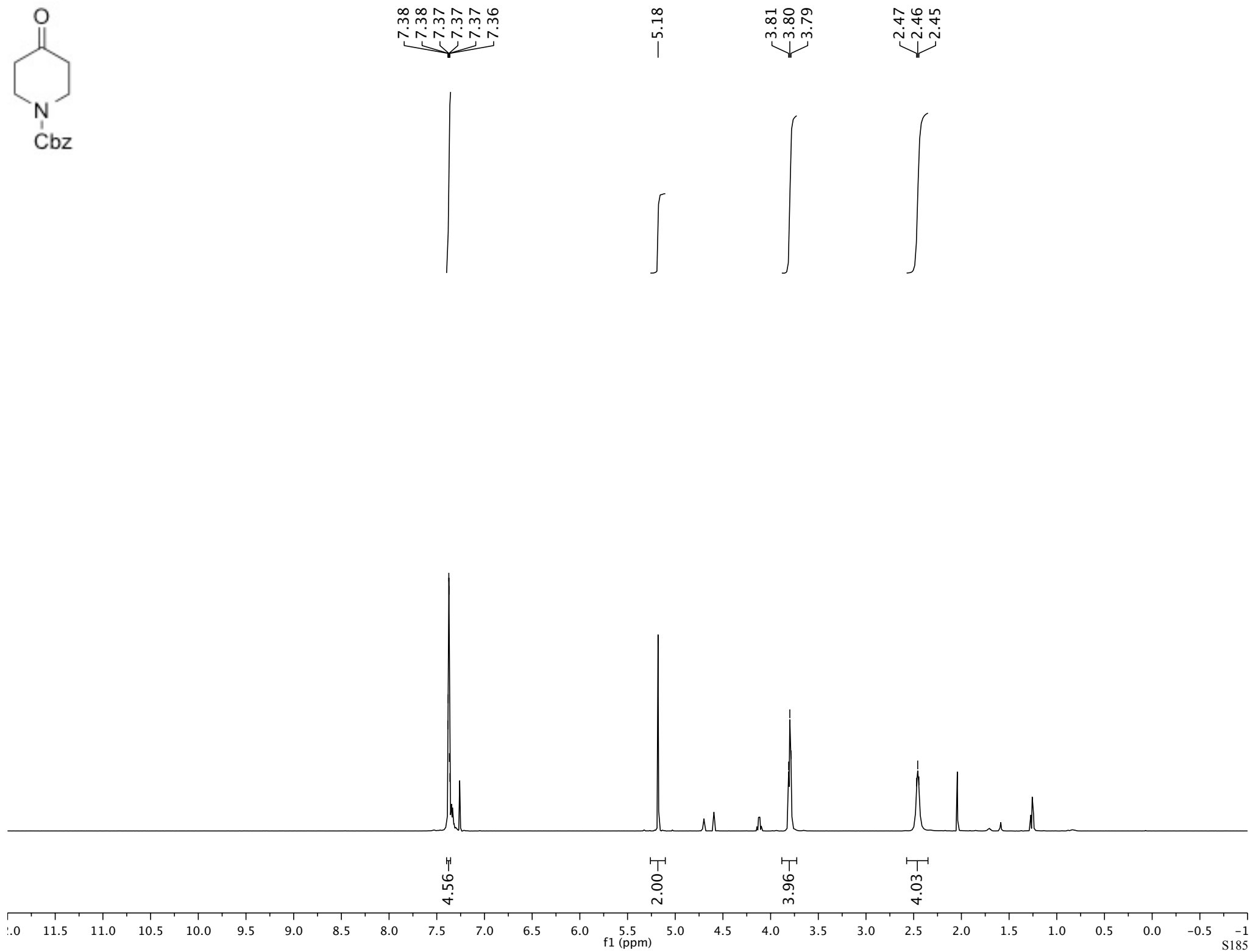
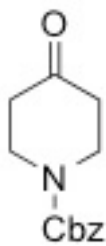
—22.58

—14.44

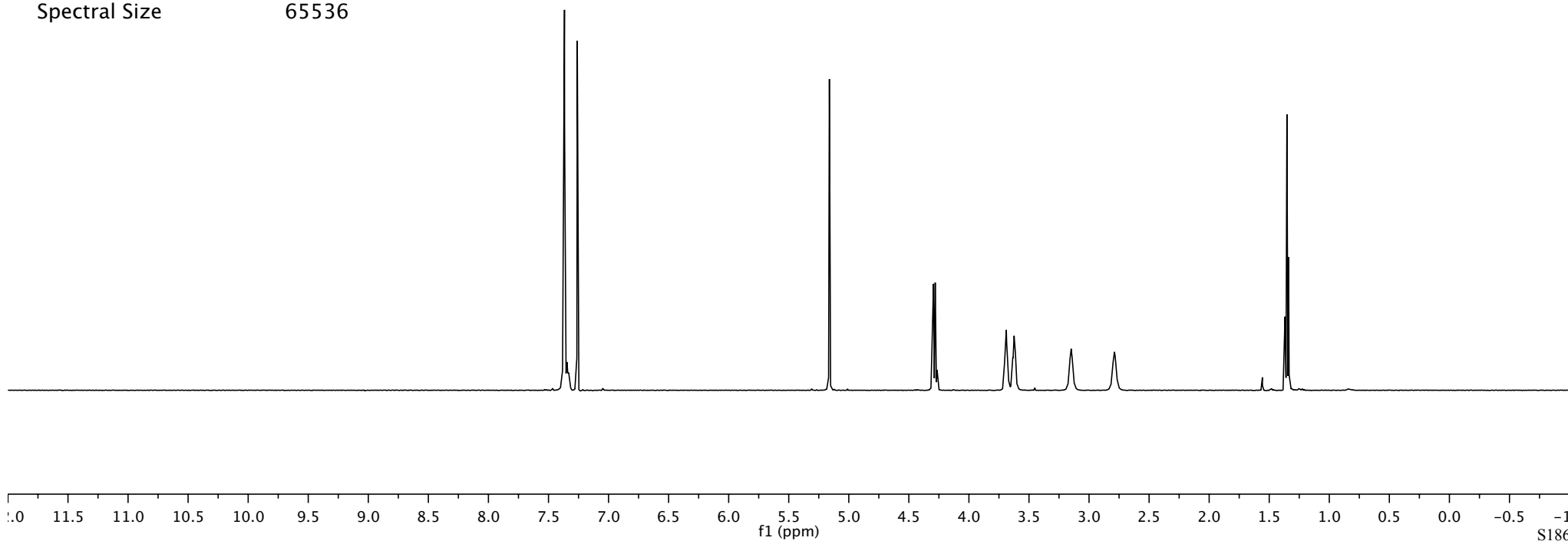
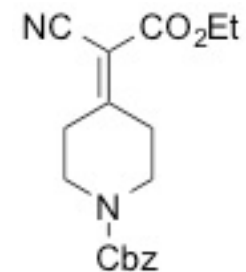


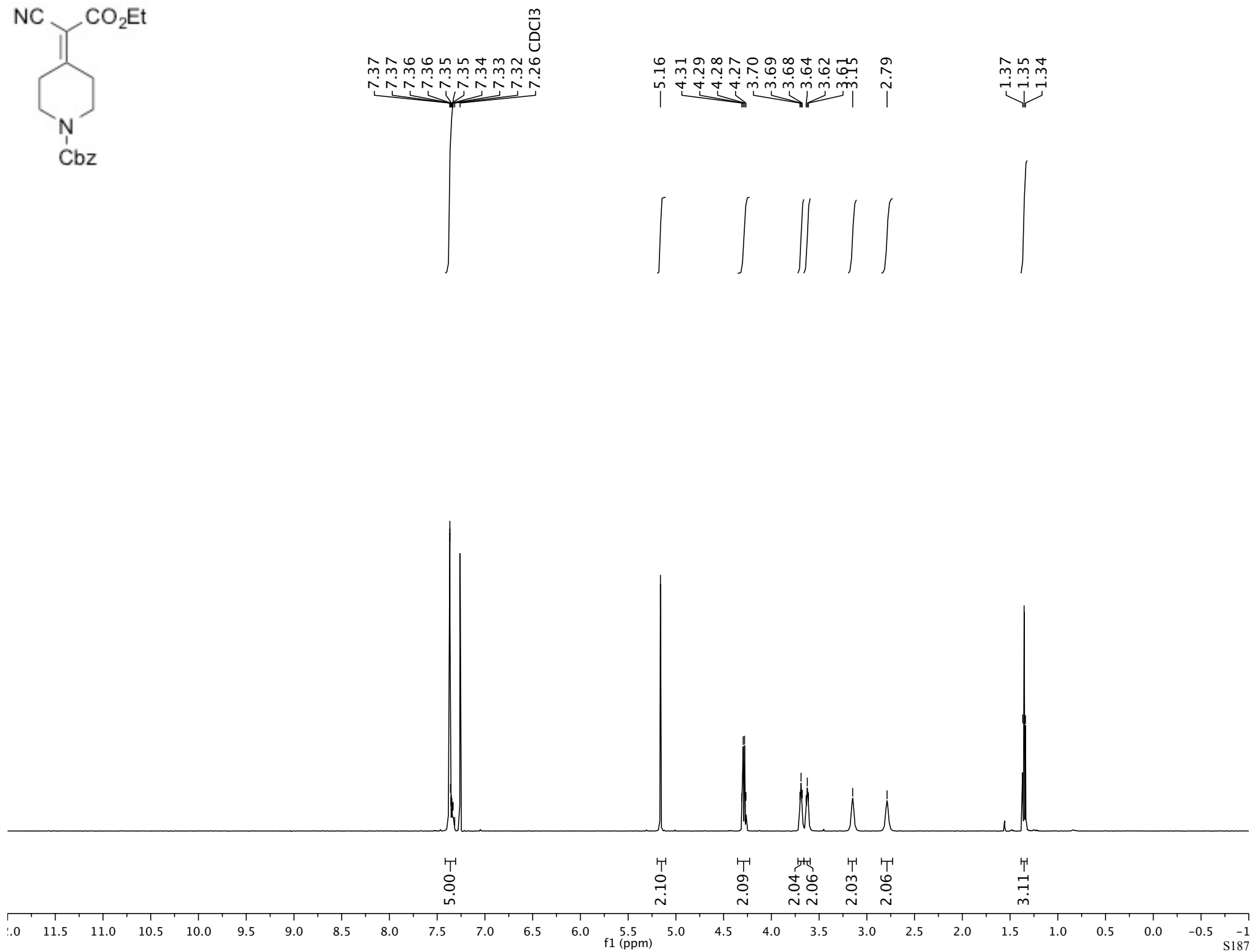
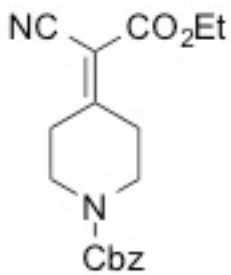
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	8
Receiver Gain	36
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1510.6
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



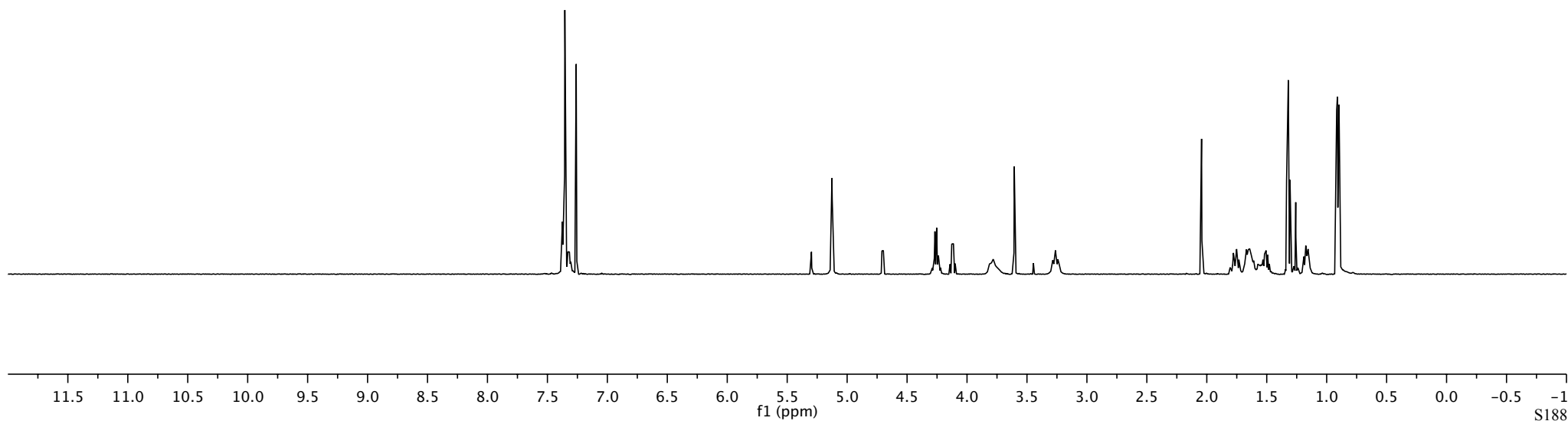
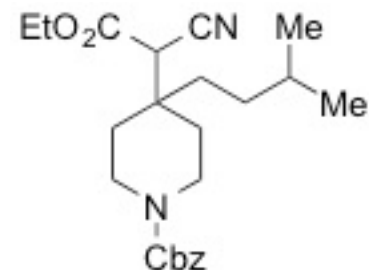


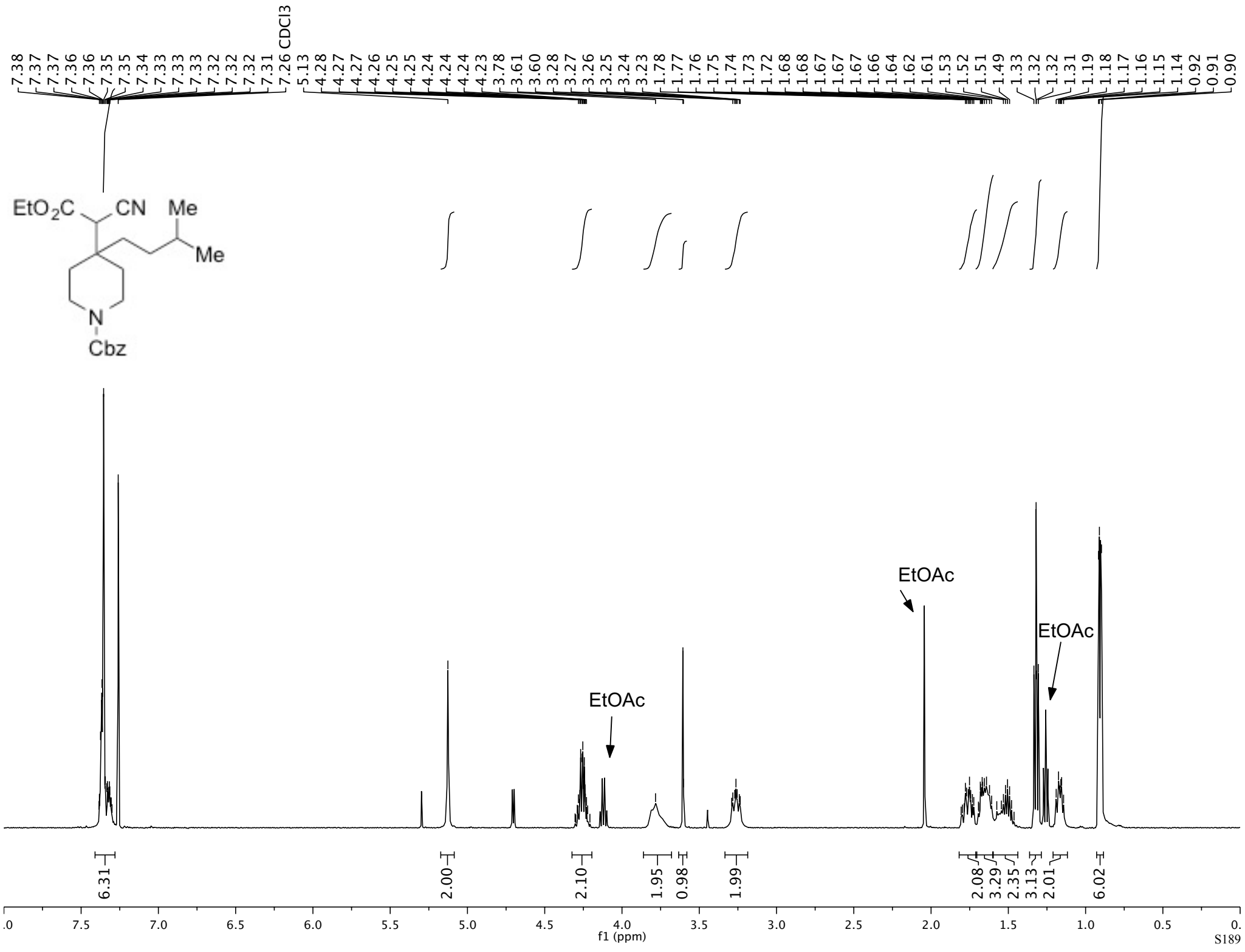
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	16
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.69
Spectral Width	7024.9
Lowest Frequency	-1011.4
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



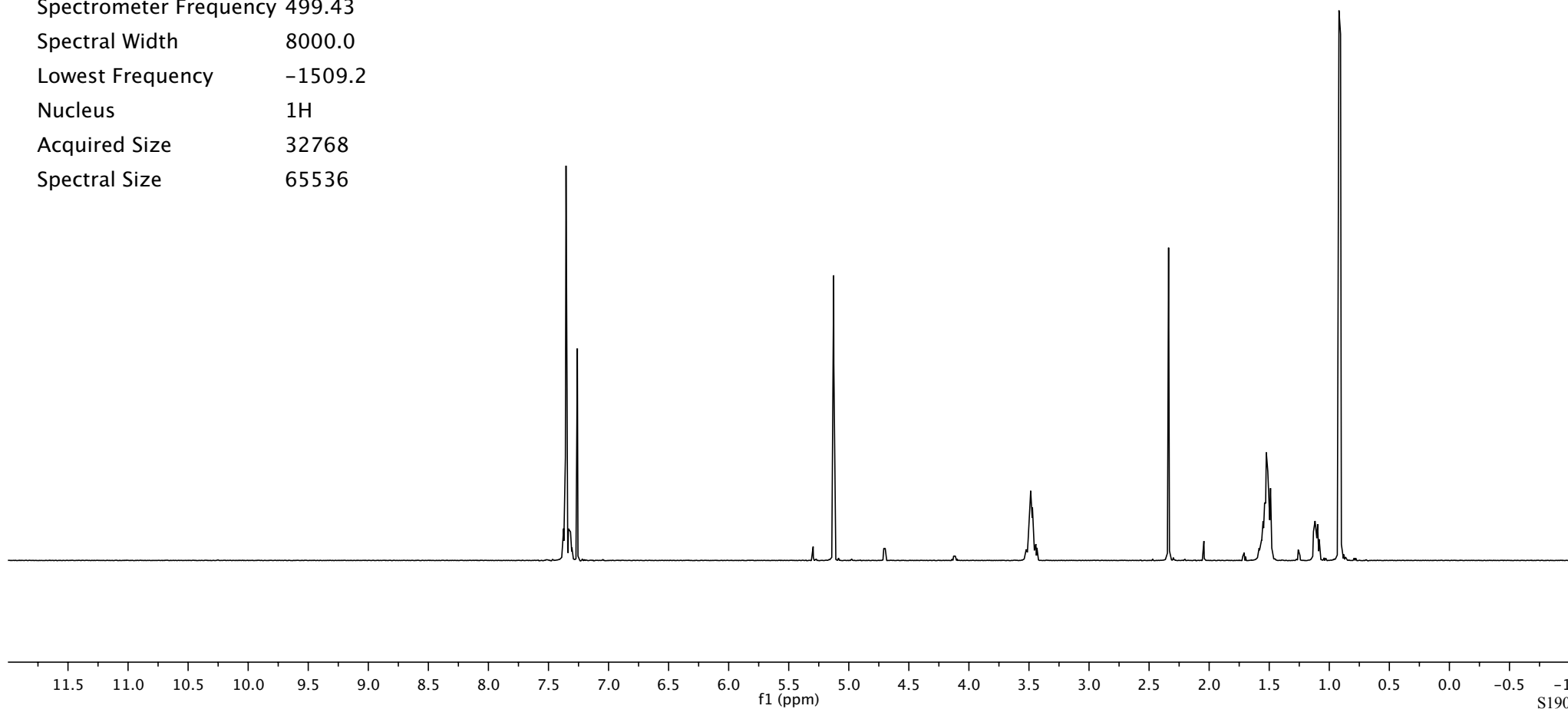
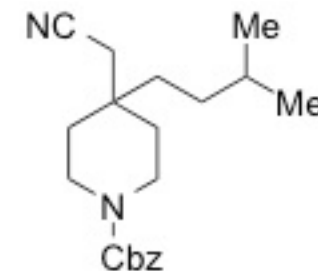


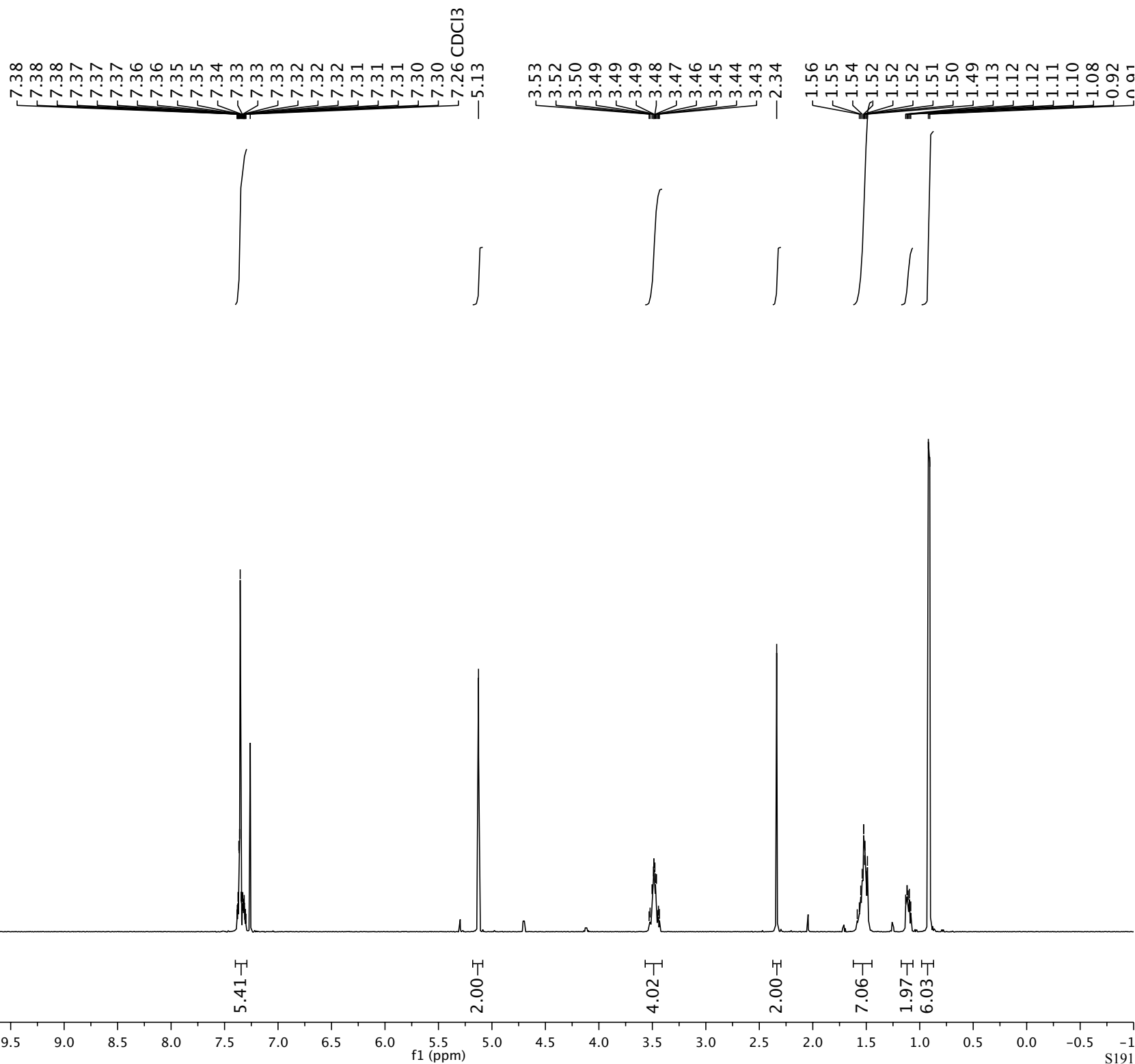
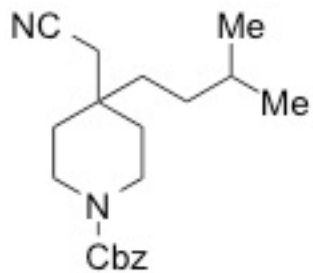
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Number of Scans	16
Receiver Gain	56
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	499.43
Spectral Width	8000.0
Lowest Frequency	-1509.2
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



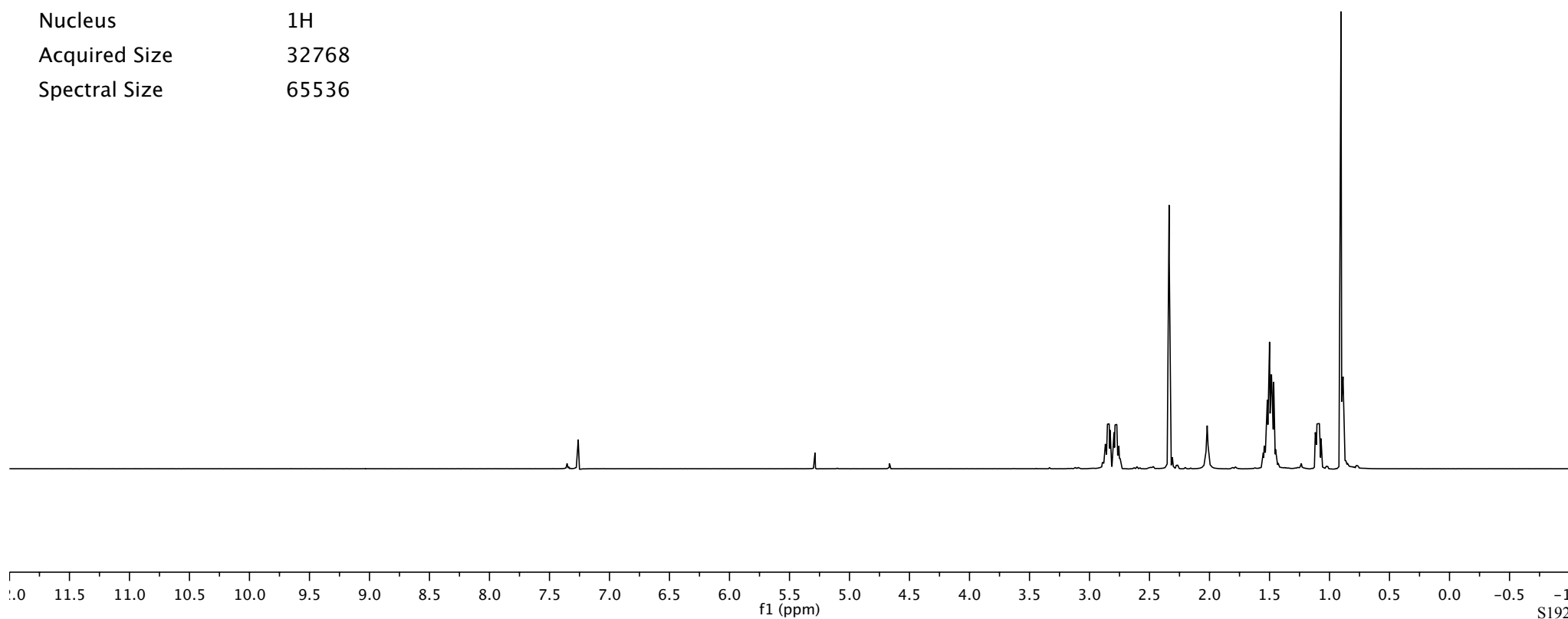
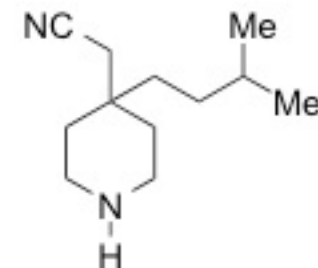


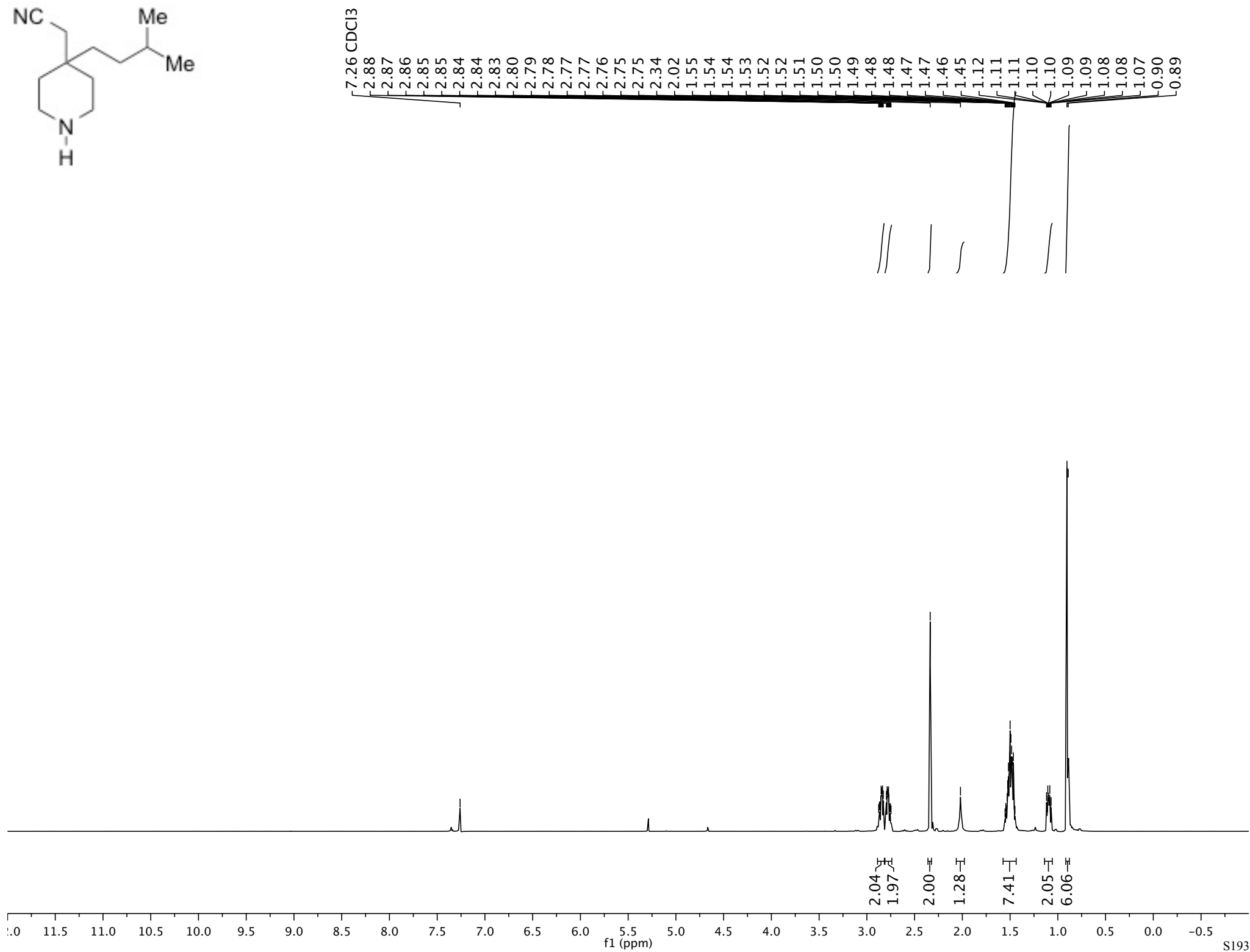
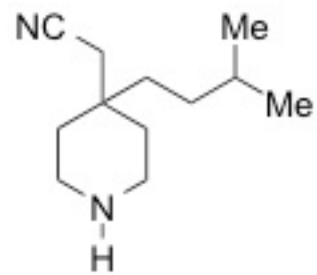
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Number of Scans	16
Receiver Gain	56
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	499.43
Spectral Width	8000.0
Lowest Frequency	-1509.2
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



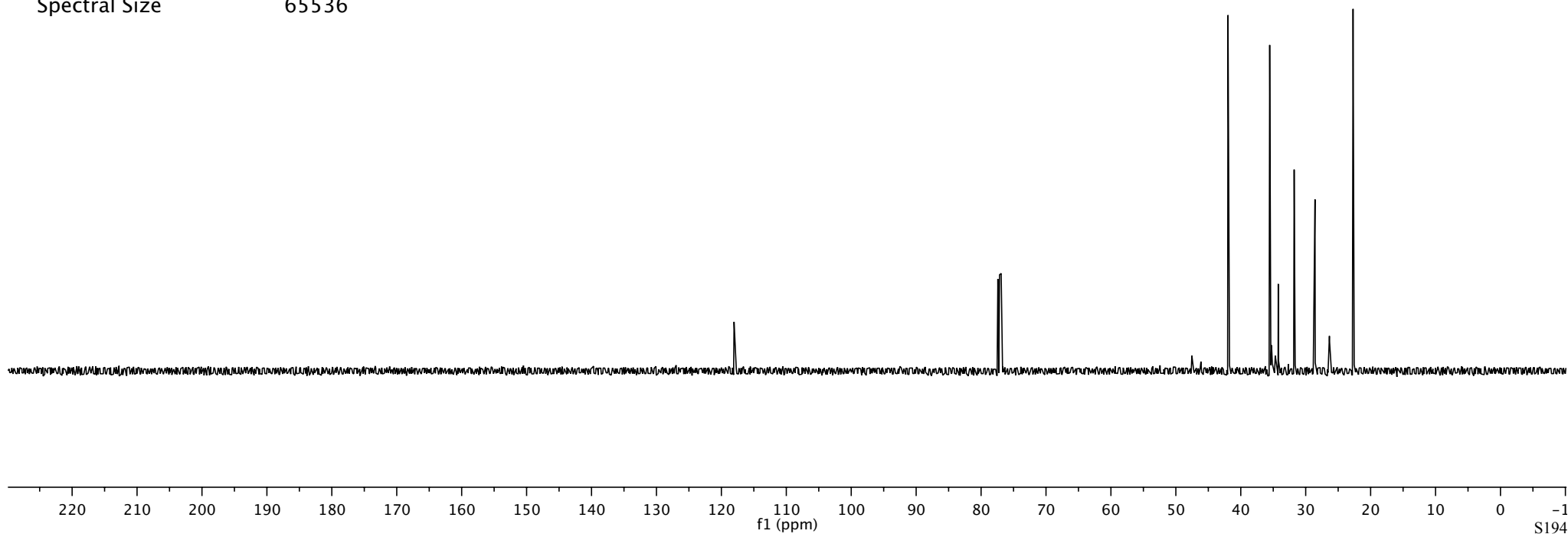
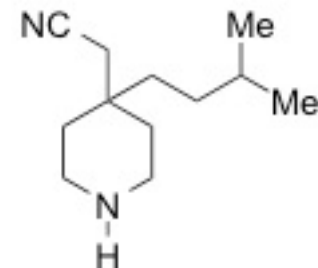


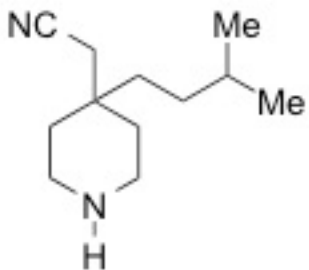
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	8
Receiver Gain	41
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.69
Spectral Width	7024.9
Lowest Frequency	-1021.9
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536





Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	128
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1277.6
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

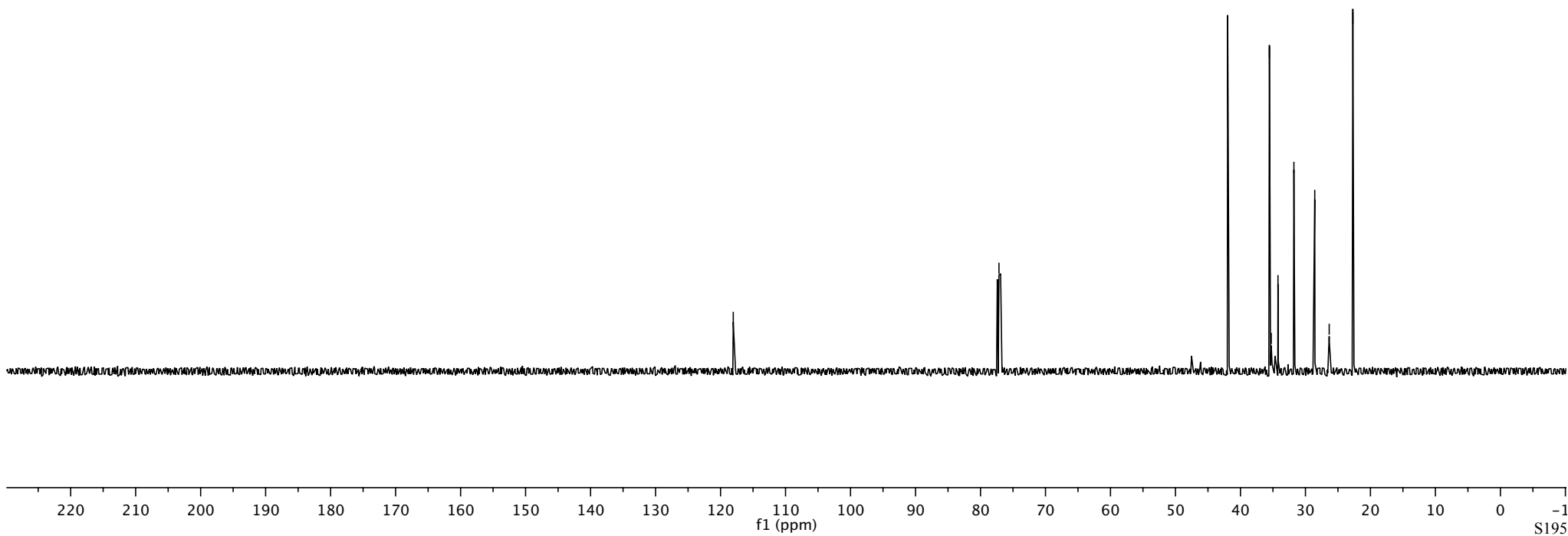




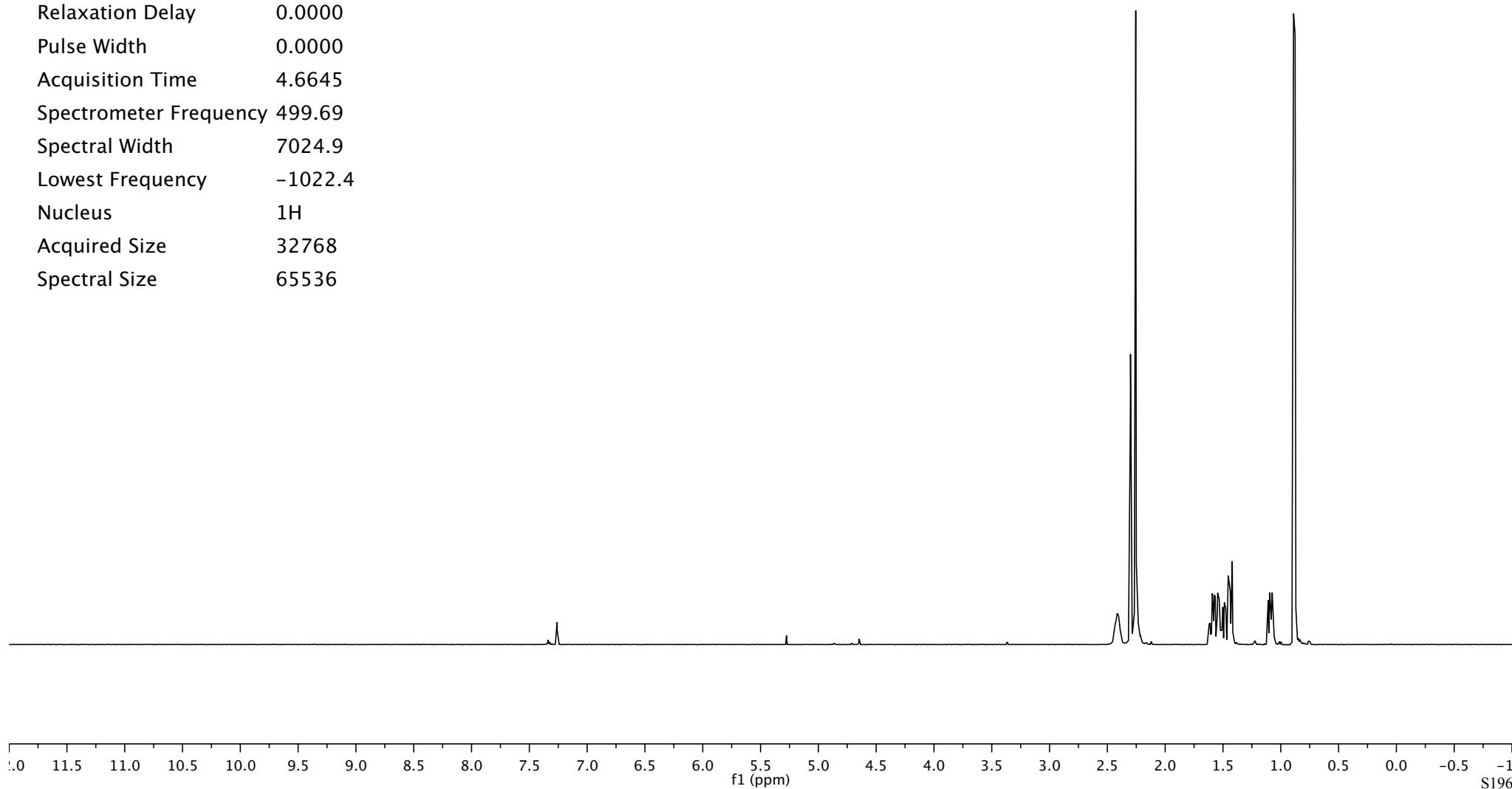
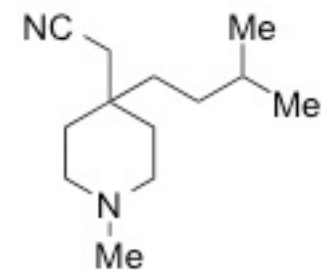
—118.04

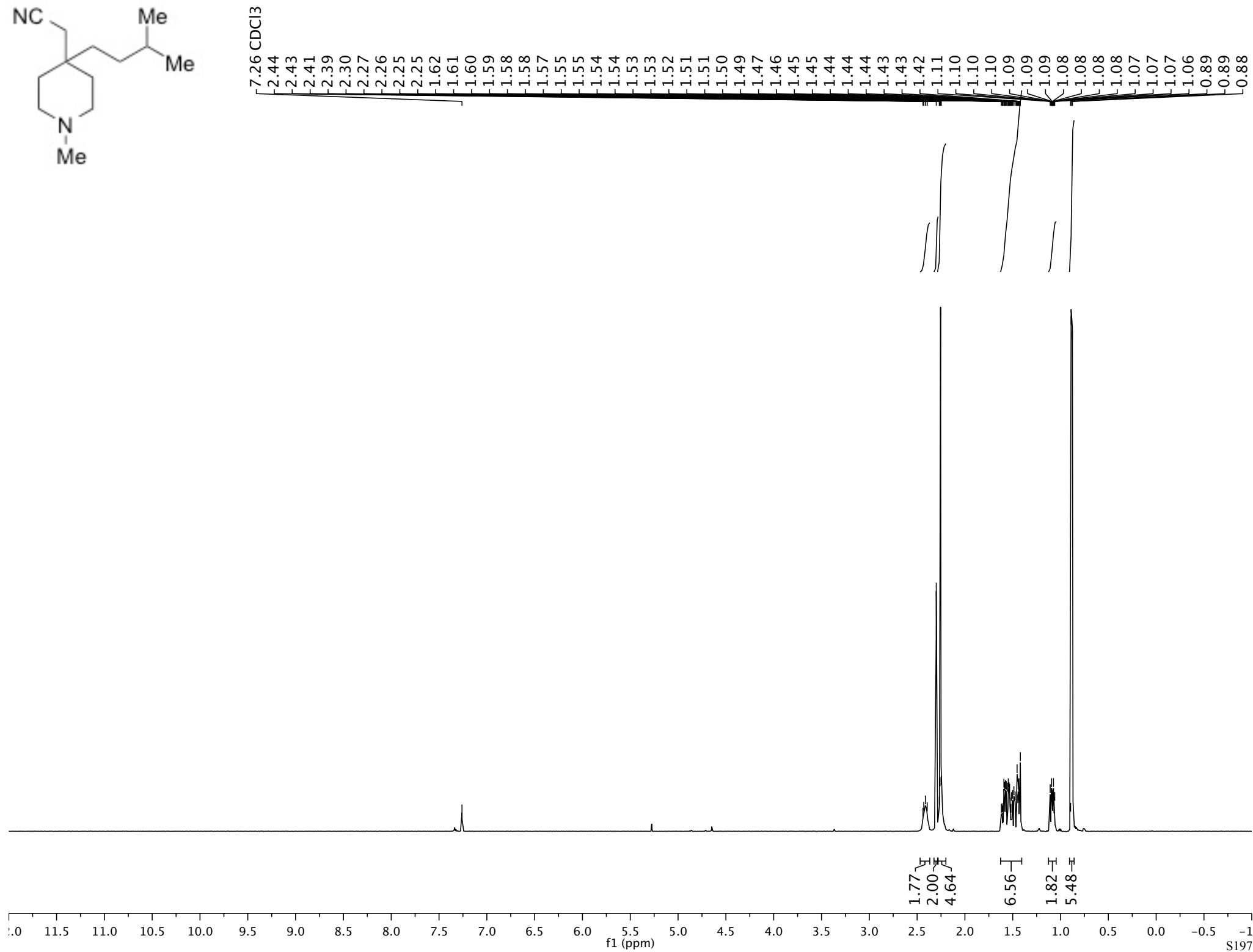
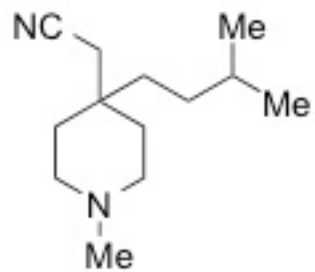
—77.16 CDCl₃

41.97
35.54
35.26
34.23
31.78
28.57
26.34
22.70

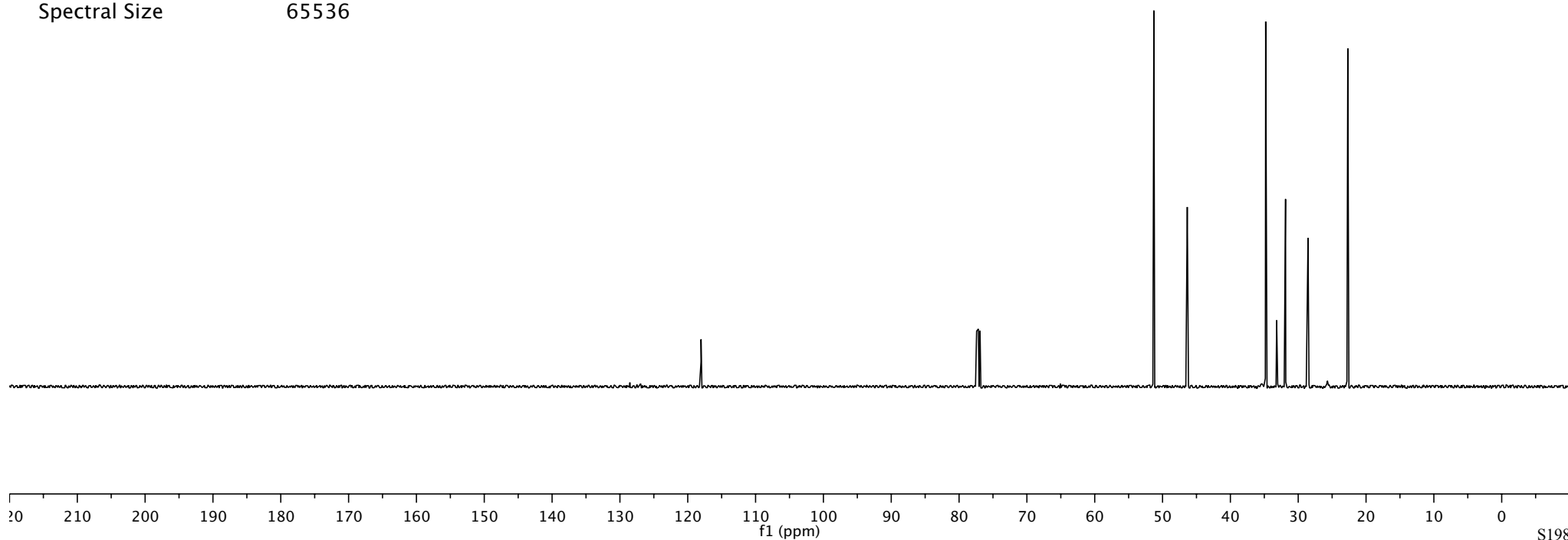
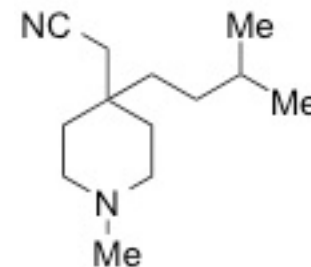


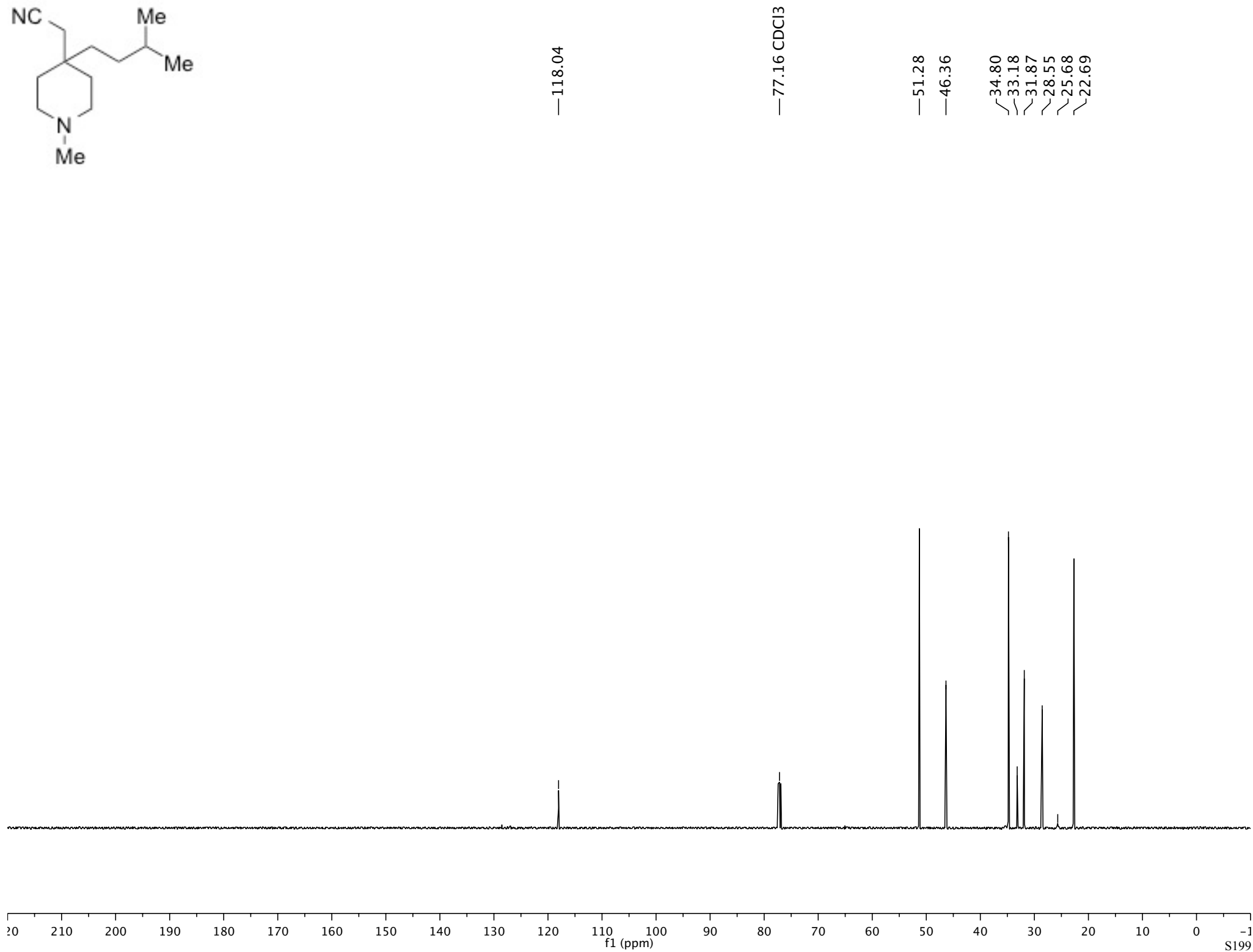
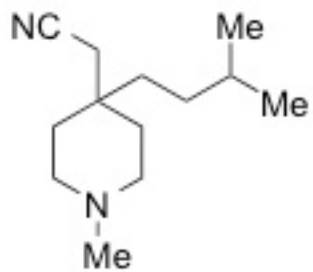
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	8
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.69
Spectral Width	7024.9
Lowest Frequency	-1022.4
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



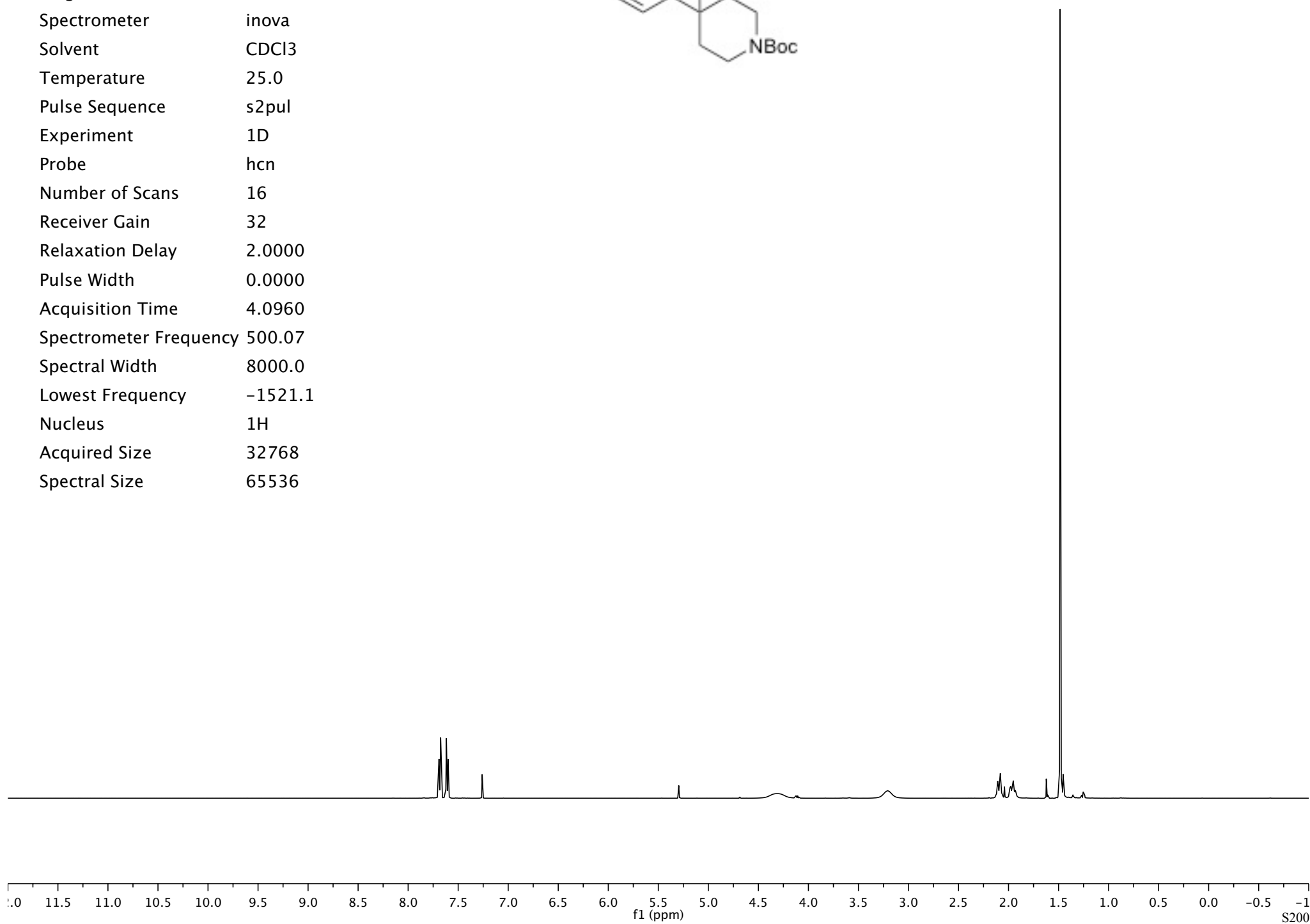
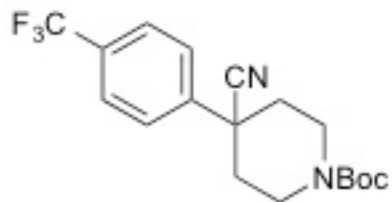


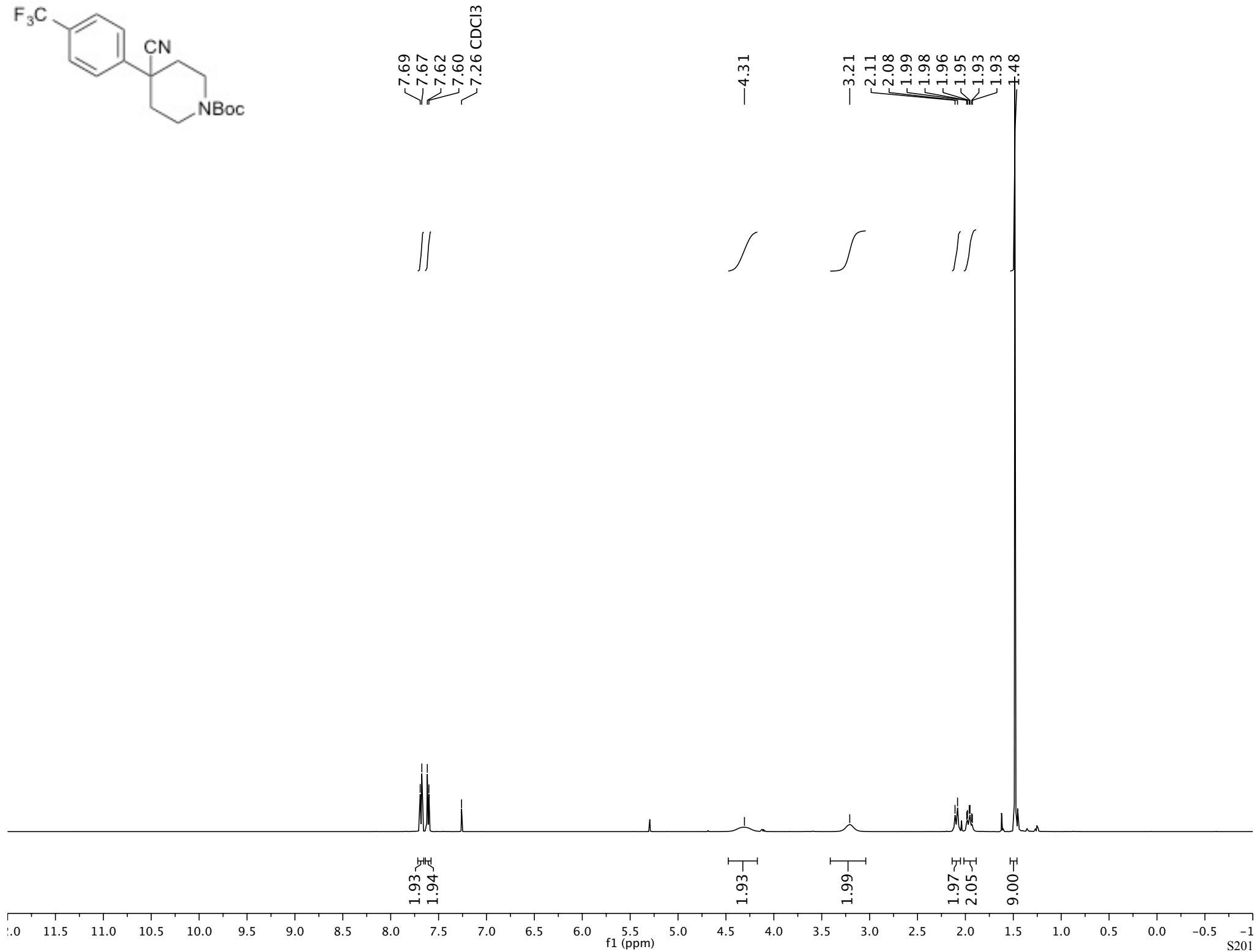
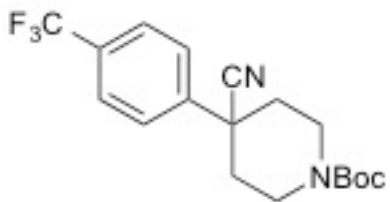
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	432
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1278.8
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

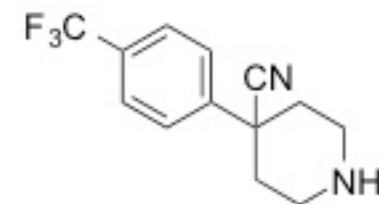




Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	32
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

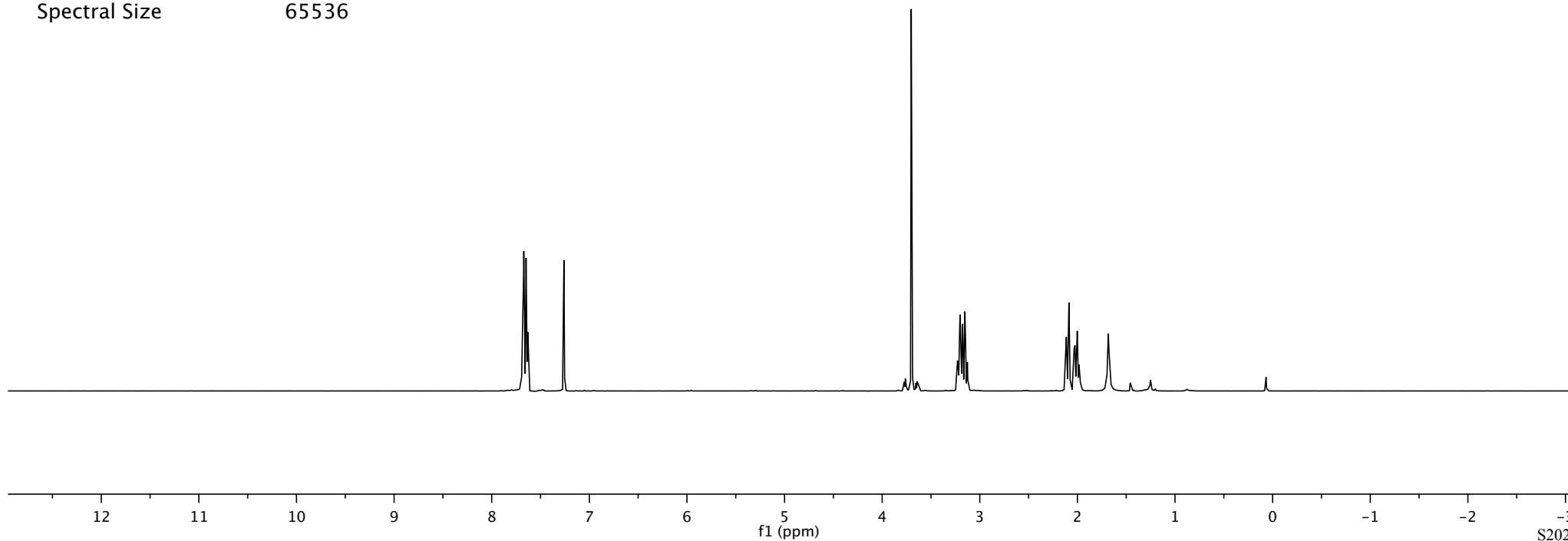


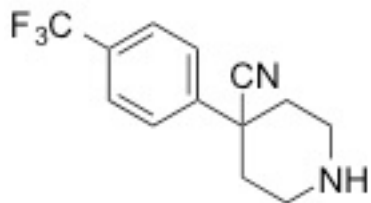




Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	42
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

1,4-dioxane

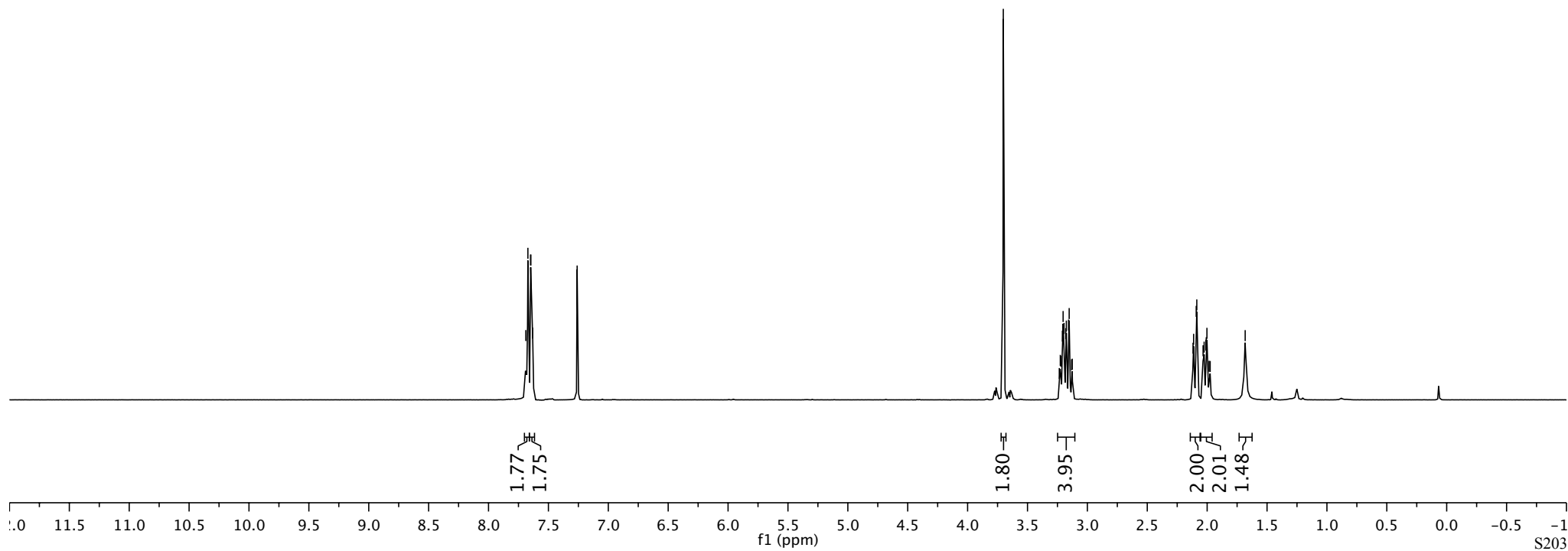




7.69
7.67
7.65
7.65
7.63
7.26 CDCl₃

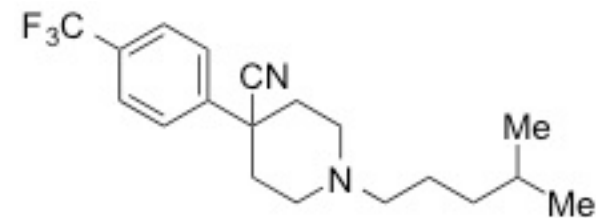
3.70
3.23
3.23
3.22
3.21
3.20
3.19
3.18
3.18
3.16
3.15
3.13
3.13
2.12
2.11
2.09
2.09
2.03
2.03
2.01
2.01
2.00
1.98
1.97
1.68

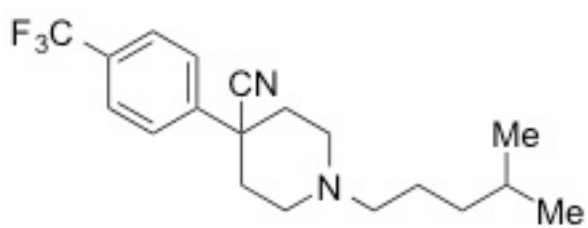
1,4-dioxane



Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

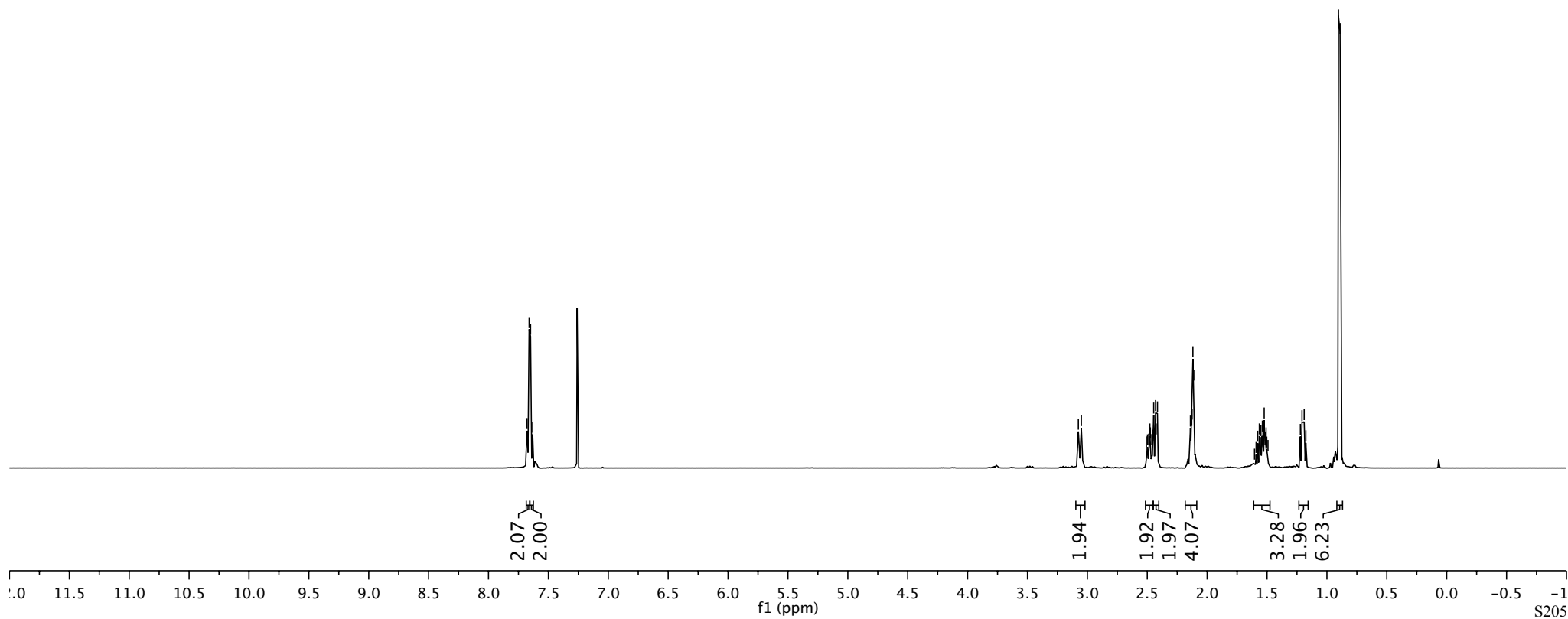
The ¹H NMR spectrum (400 MHz, CDCl₃) of compound 10a shows several characteristic peaks. Aromatic protons appear as a multiplet between 7.2 and 7.8 ppm. A sharp singlet at approximately 7.7 ppm corresponds to the aldehyde proton. The aliphatic region (1.0 to 3.0 ppm) contains several multiplets and singlets, including a prominent singlet at 1.0 ppm (likely a methyl group) and a sharp singlet at 2.1 ppm (likely an acetyl methyl group). The x-axis is labeled 'f1 (ppm)' and ranges from 12.0 to -1.0.

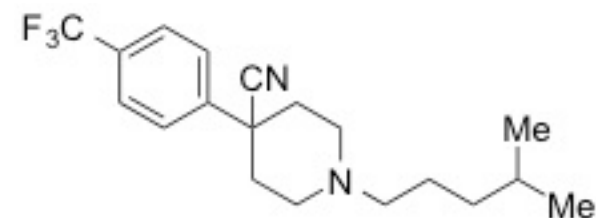




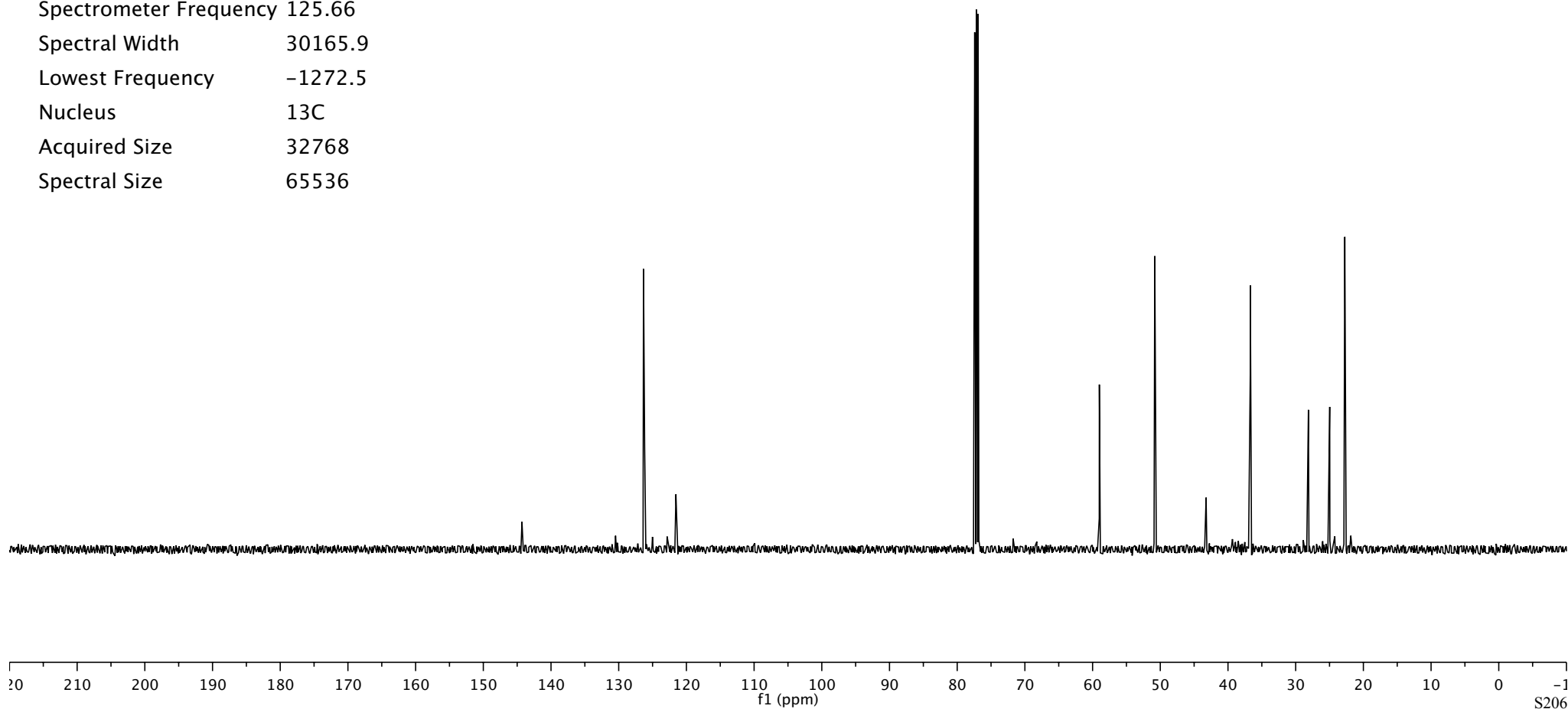
7.68
7.66
7.65
7.63
7.26 CDCl₃

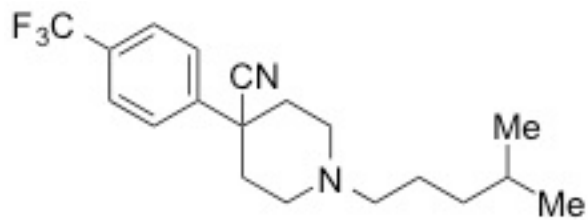
3.08
3.05
2.51
2.50
2.49
2.48
2.48
2.47
2.46
2.45
2.45
2.44
2.43
2.43
2.41
2.14
2.13
2.13
2.13
2.12
2.11
1.58
1.56
1.55
1.54
1.53
1.53
1.52
1.51
1.51
1.22
1.21
1.19
1.18
0.90
0.89





Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	1161
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1272.5
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536





— 144.29
— 130.73
— 130.47
— 126.34
— 126.22
— 126.20
— 126.17
— 126.14
— 125.01
— 122.85
— 121.55

— 77.16 CDCl₃

— 59.00

— 50.82

— 43.23

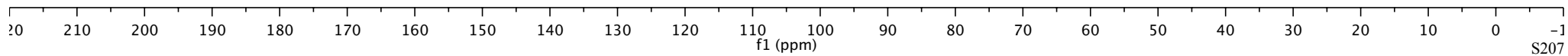
— 36.88

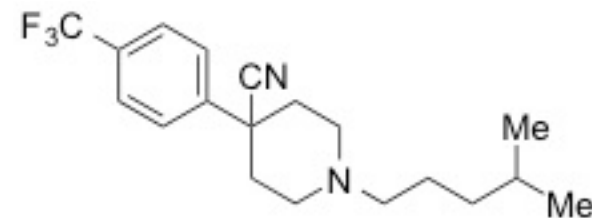
— 36.70

— 28.12

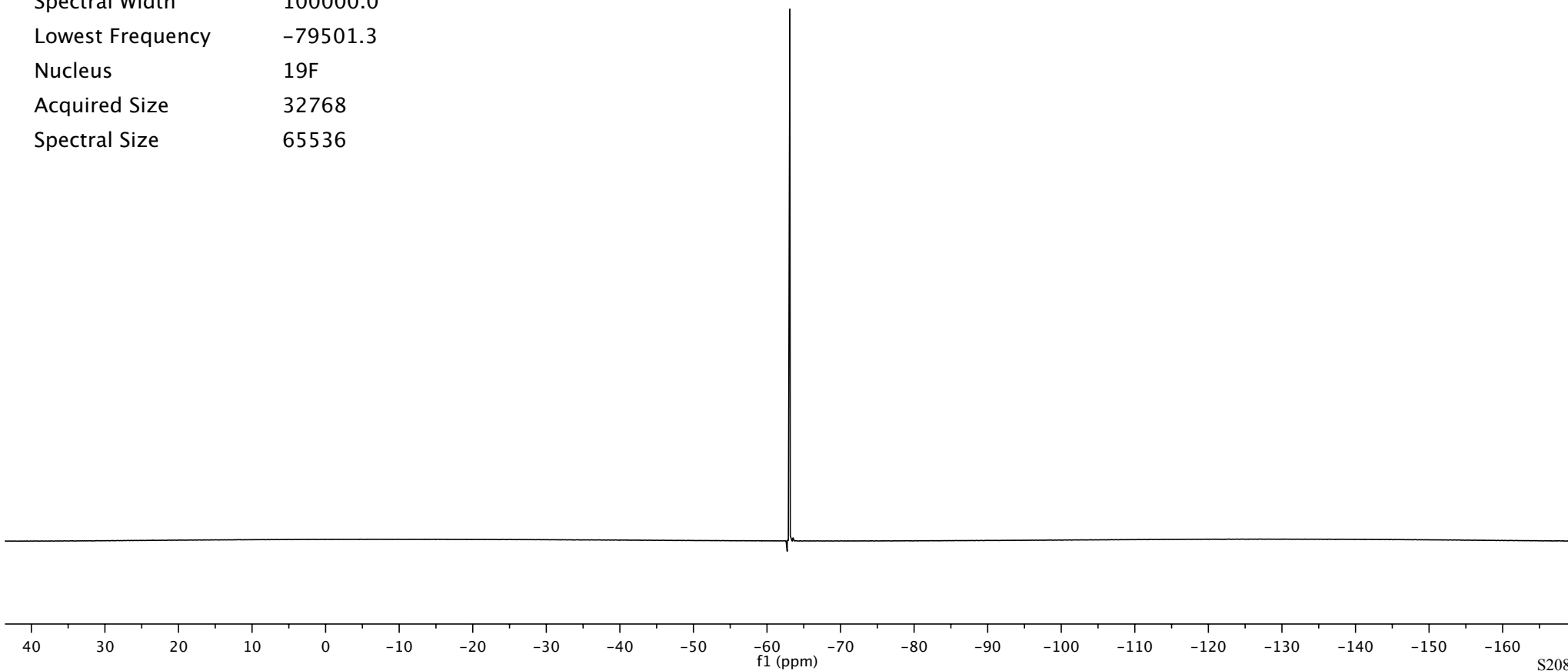
— 24.97

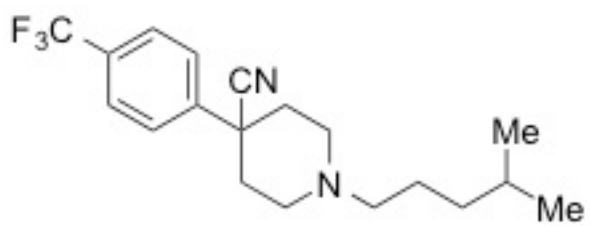
— 22.75



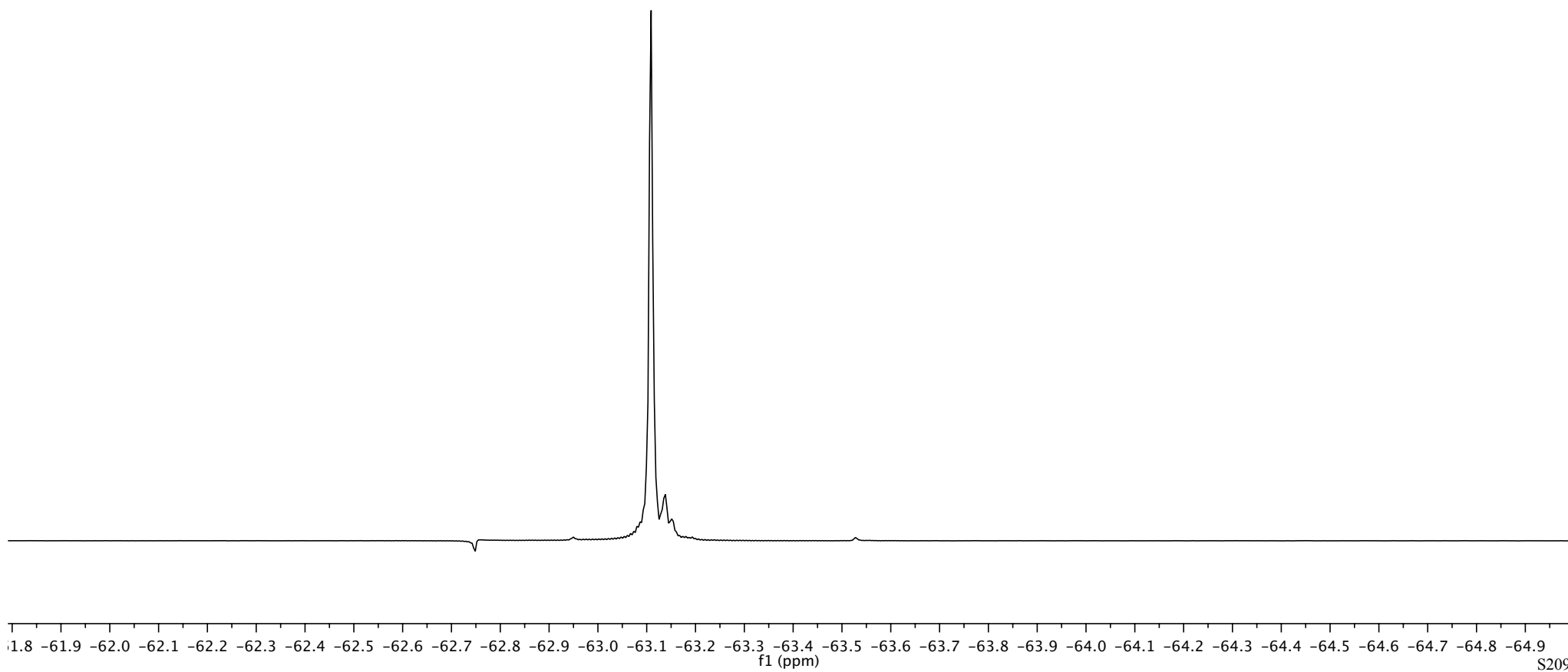


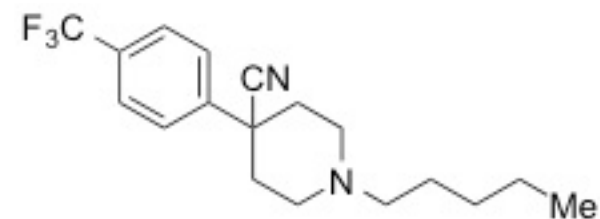
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	128
Receiver Gain	52
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency	-79501.3
Nucleus	19F
Acquired Size	32768
Spectral Size	65536



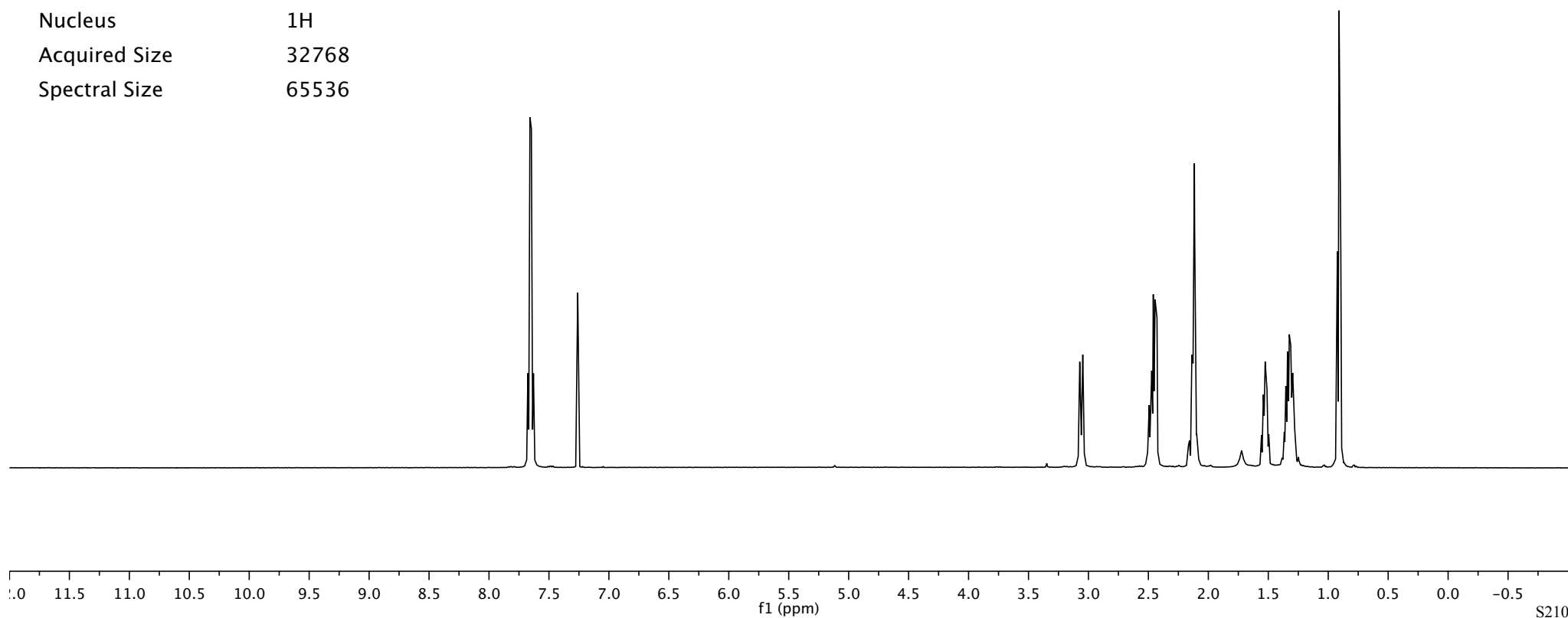


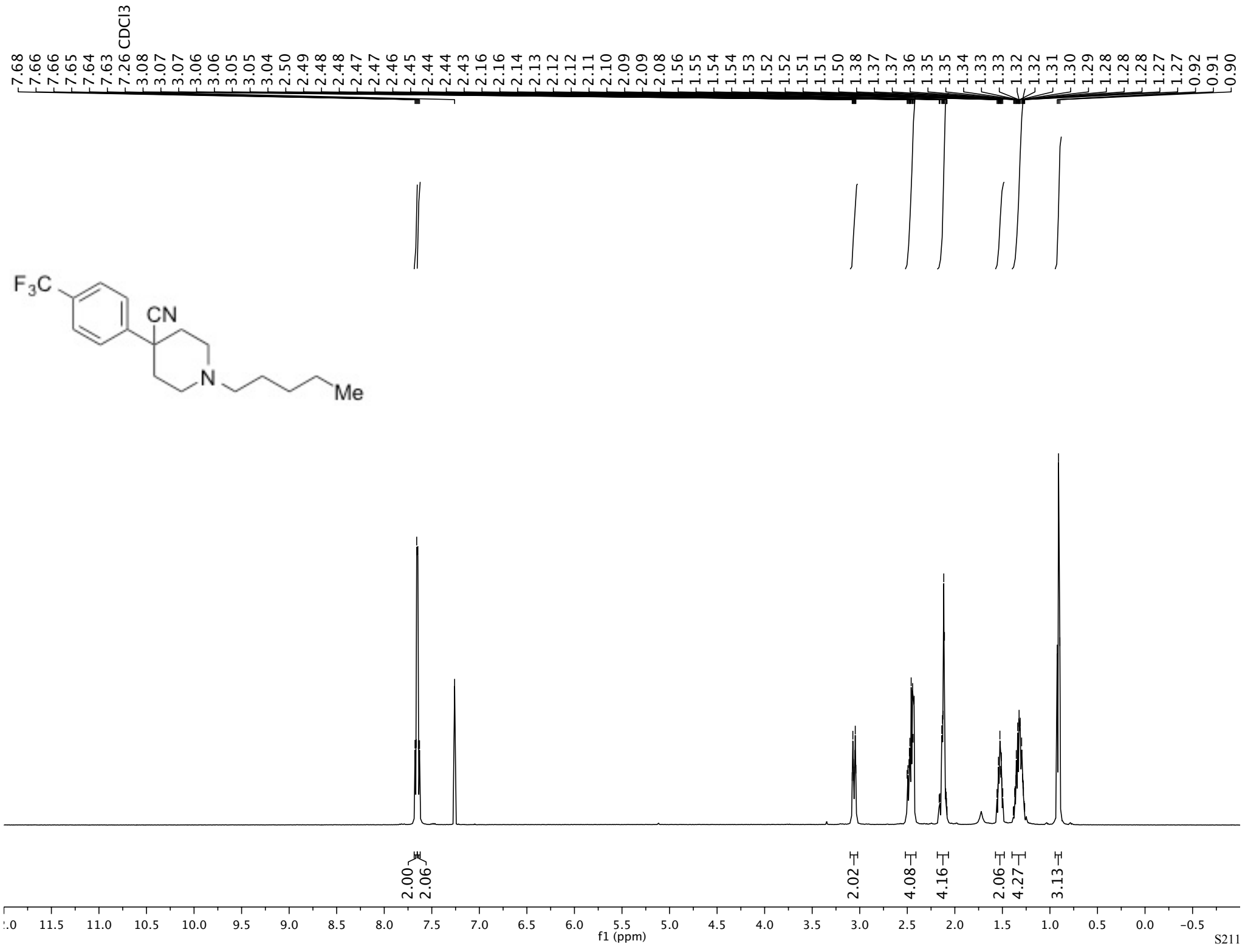
---63.11

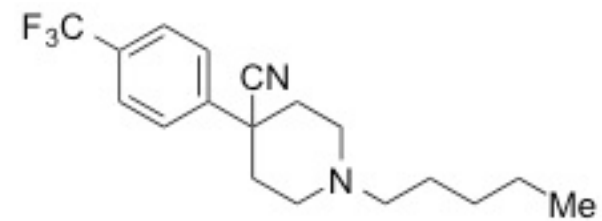




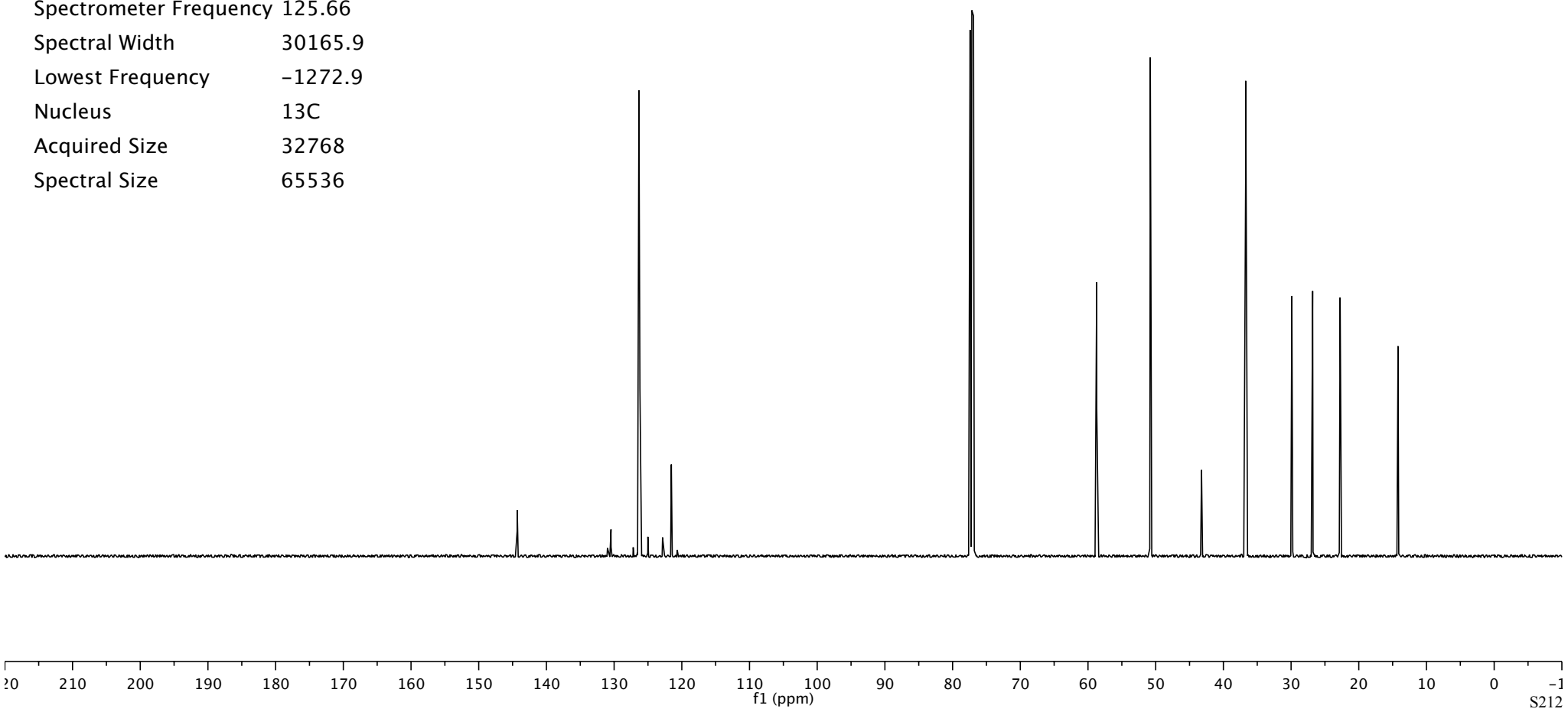
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	16
Receiver Gain	46
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.69
Spectral Width	7024.9
Lowest Frequency	-1021.9
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

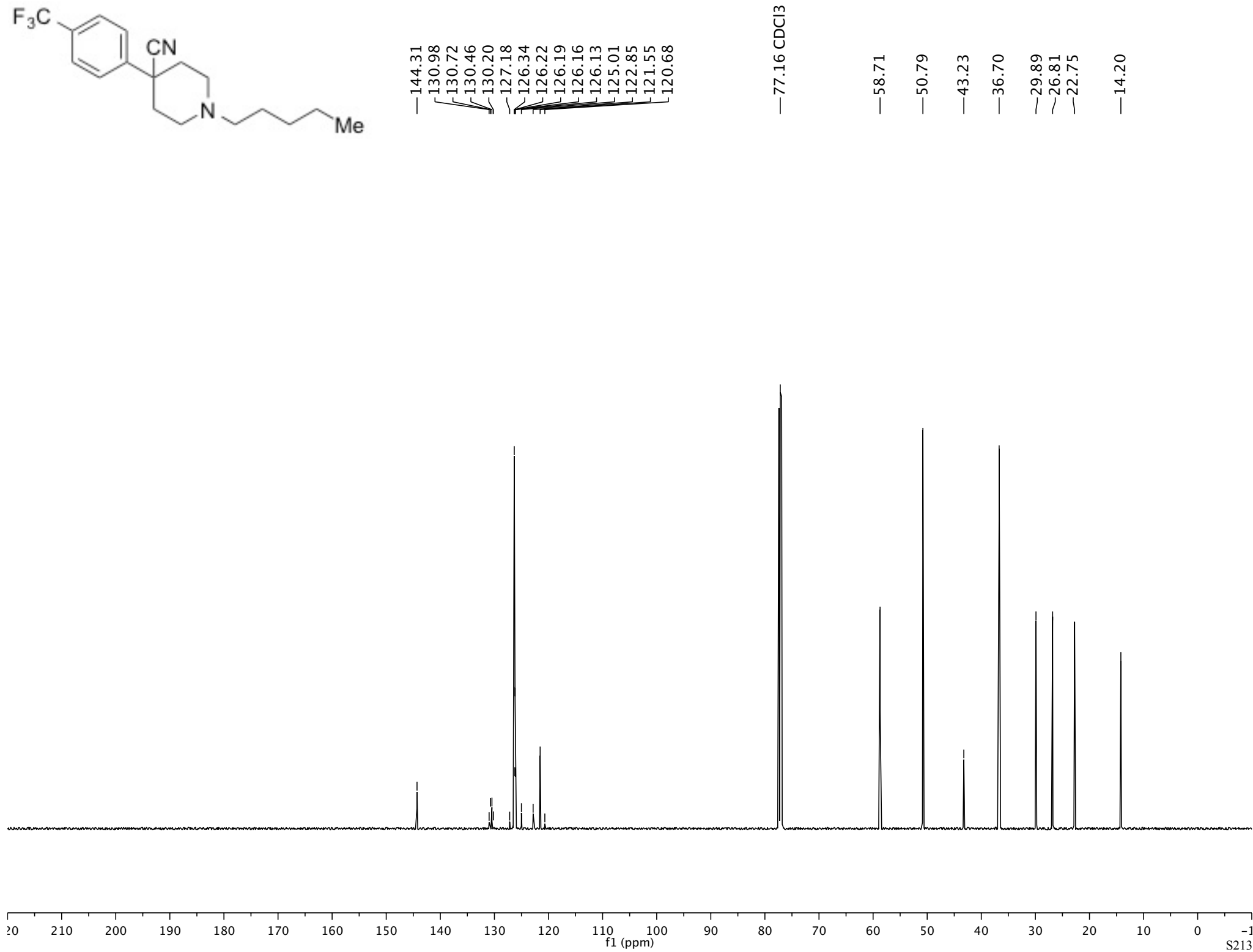
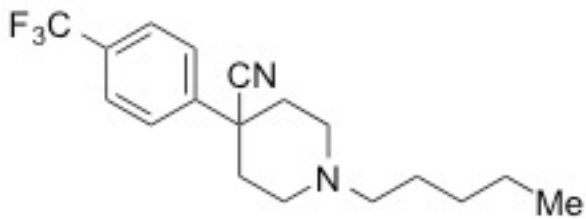




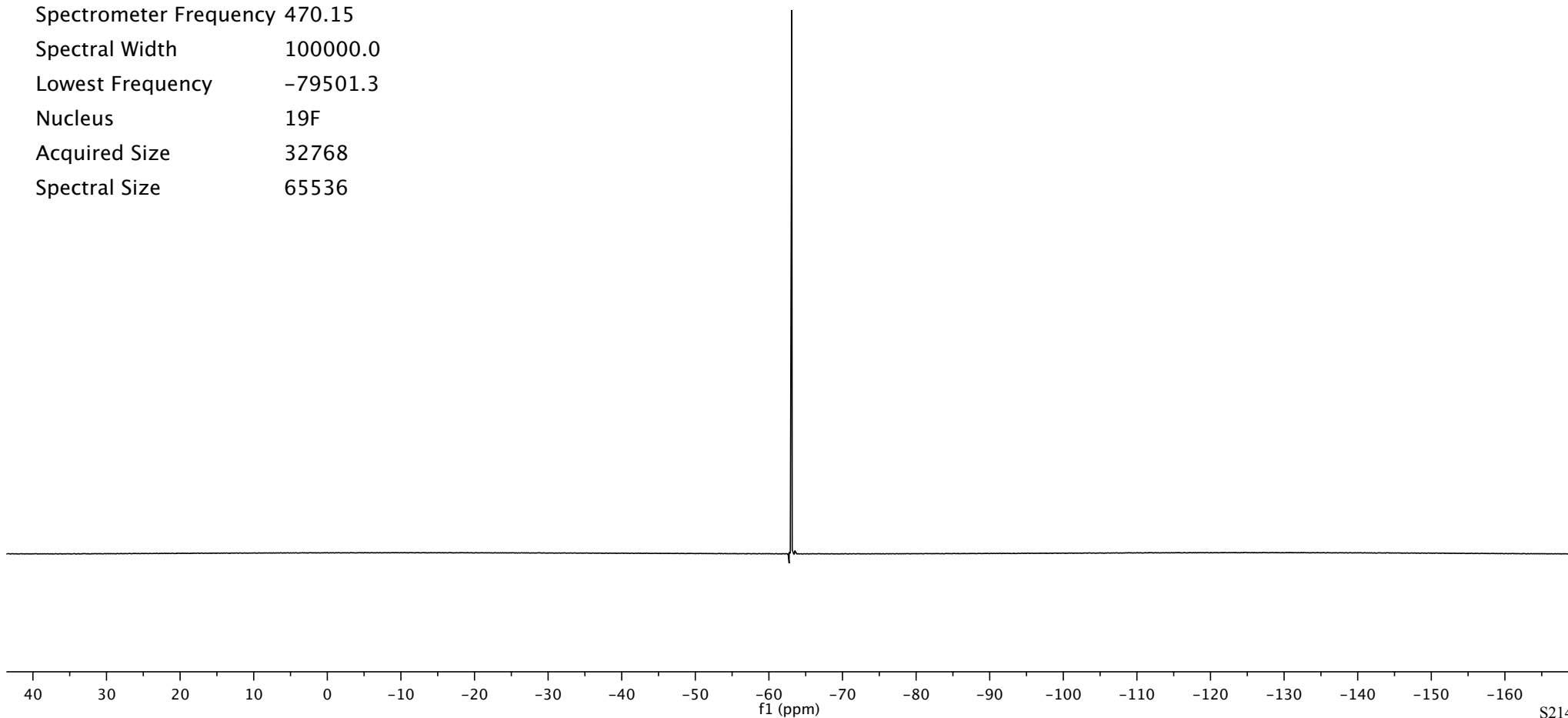
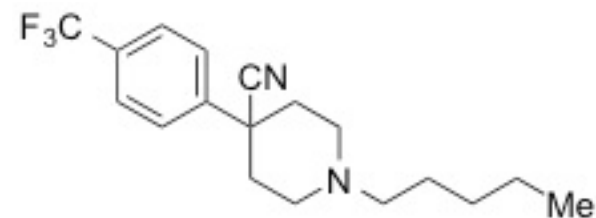


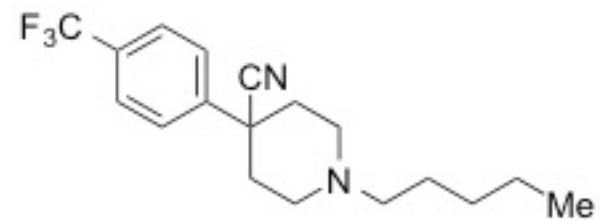
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	11512
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1272.9
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



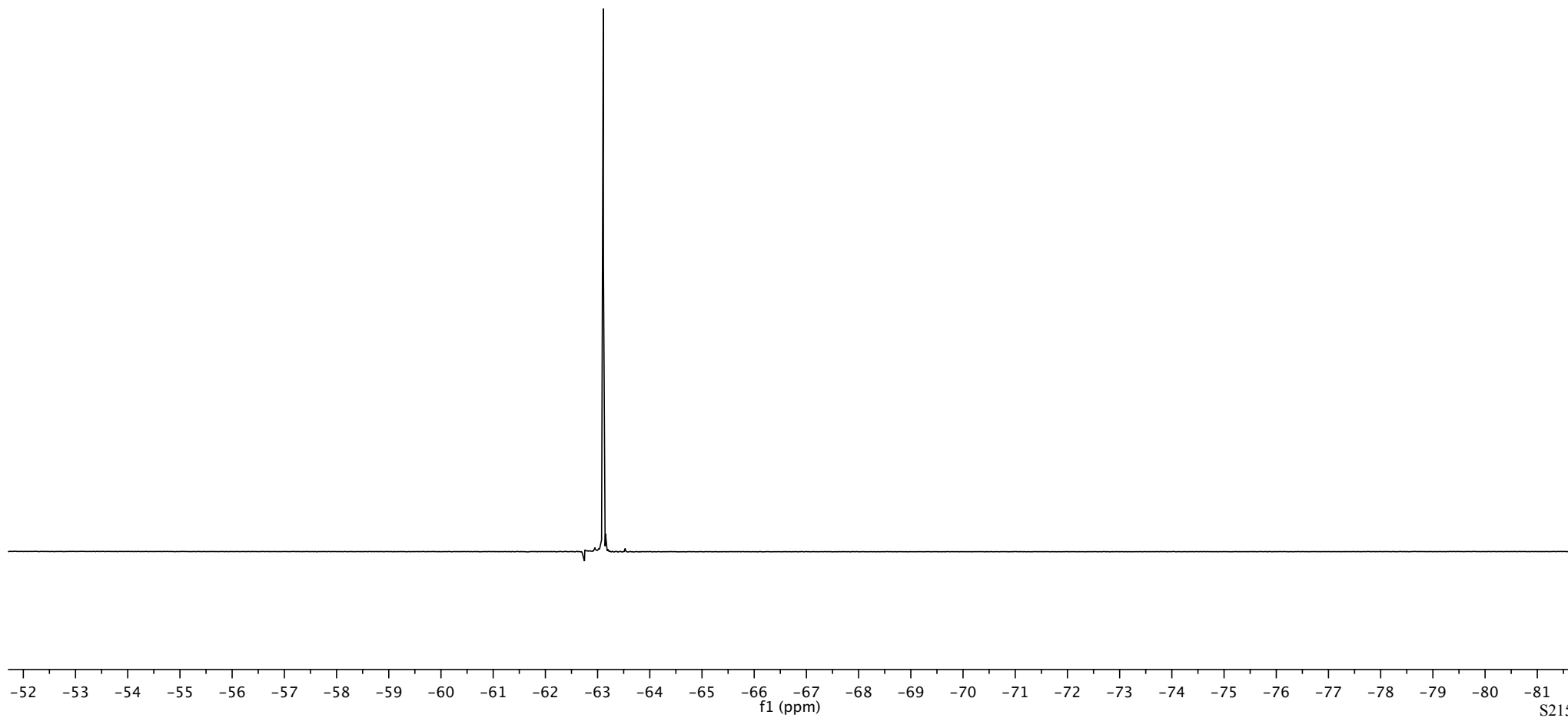


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	132
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency	-79501.3
Nucleus	19F
Acquired Size	32768
Spectral Size	65536

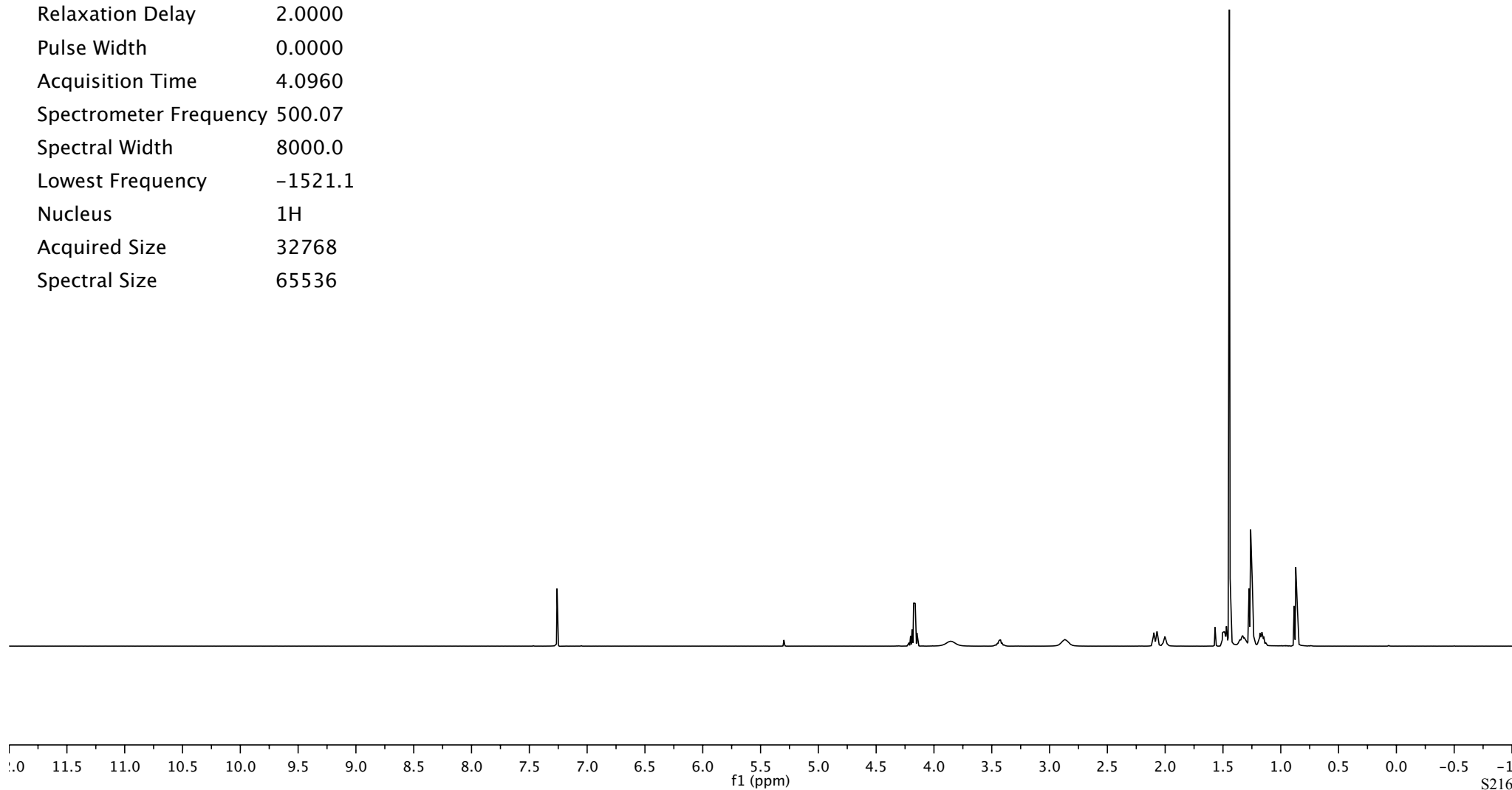
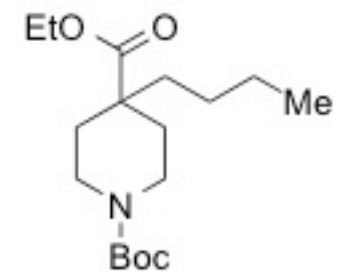


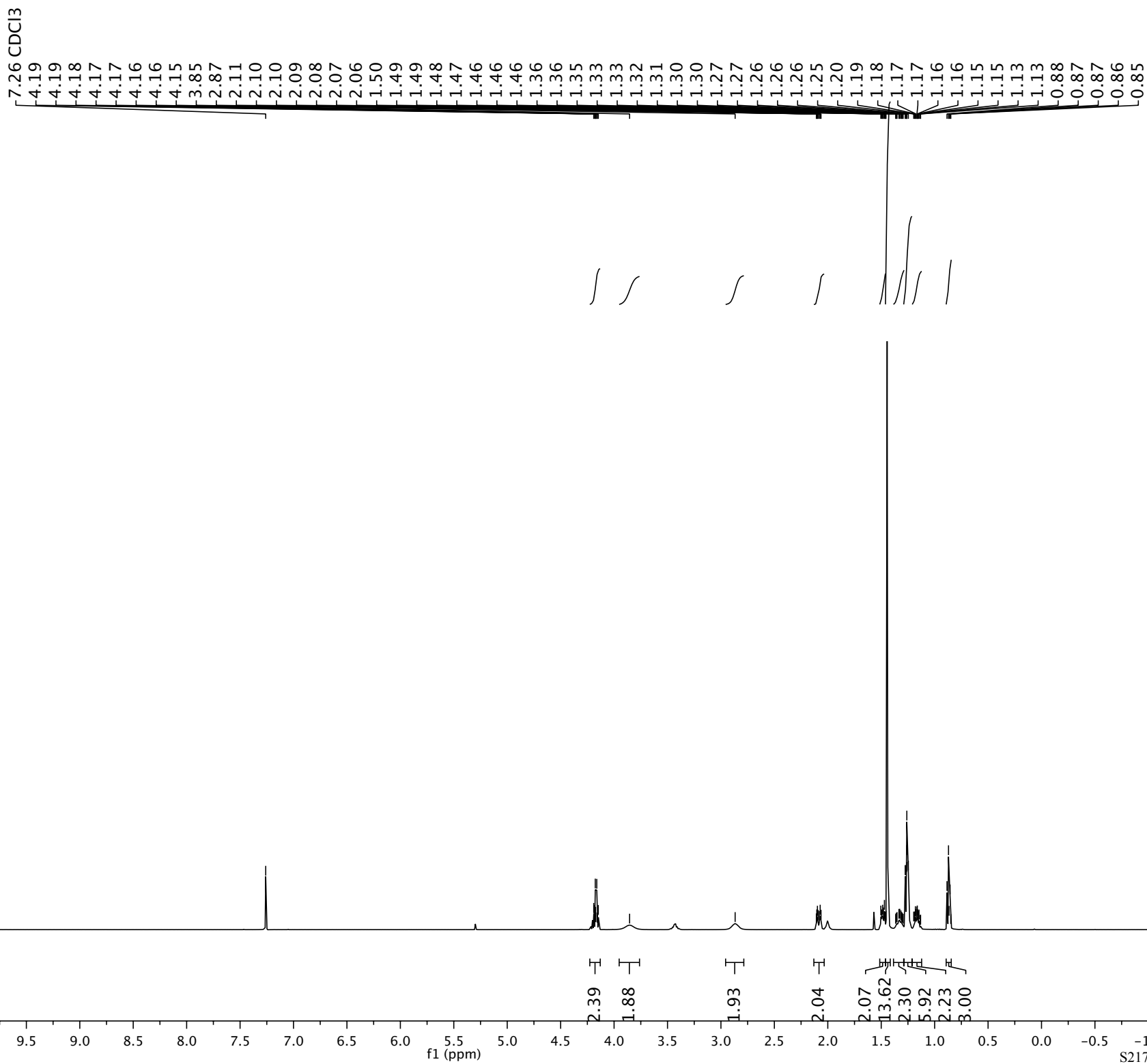
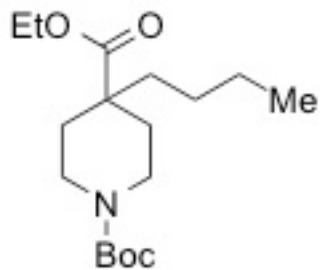


--63.11

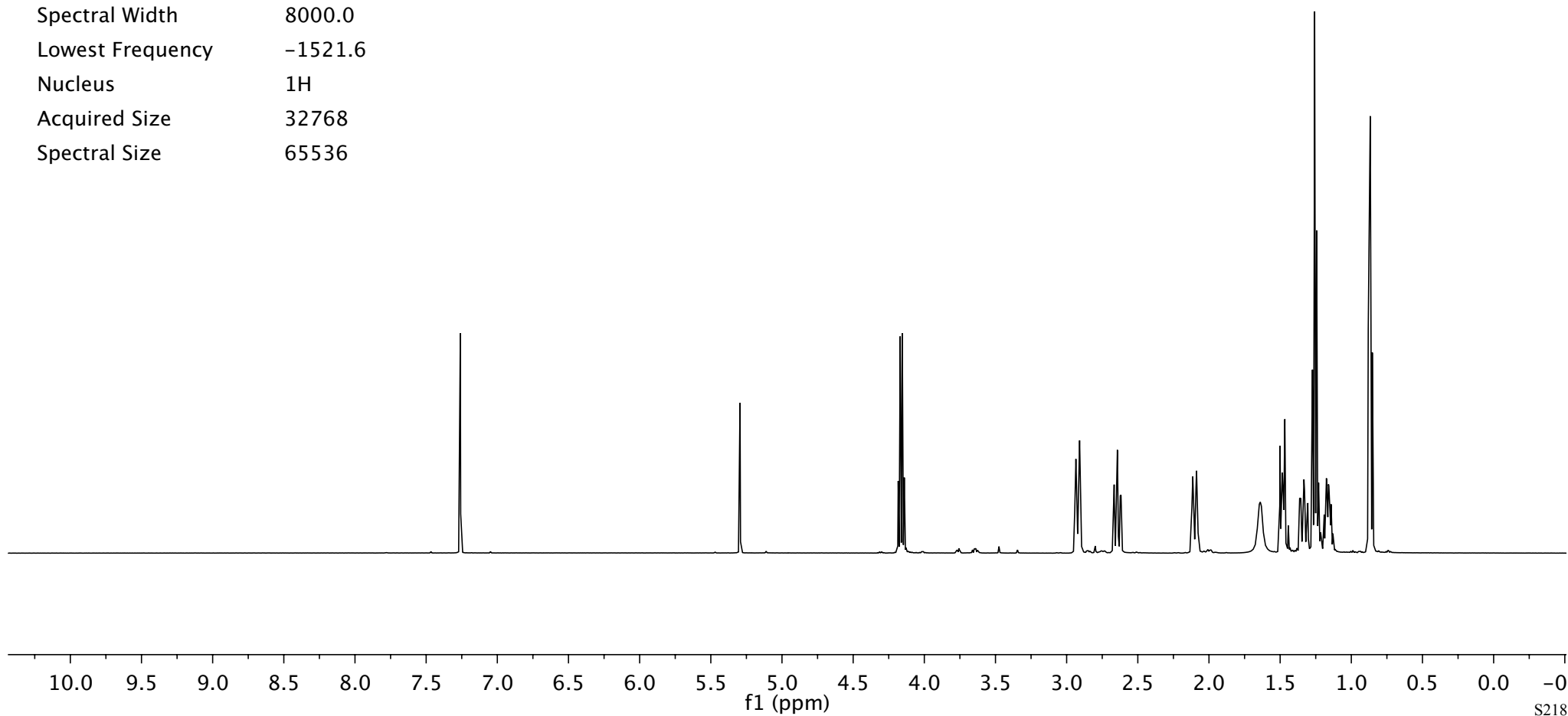
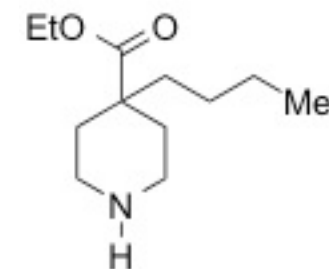


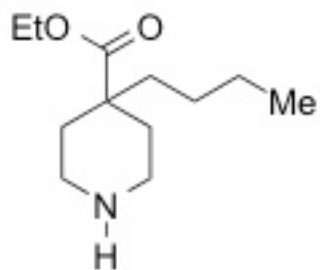
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	32
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



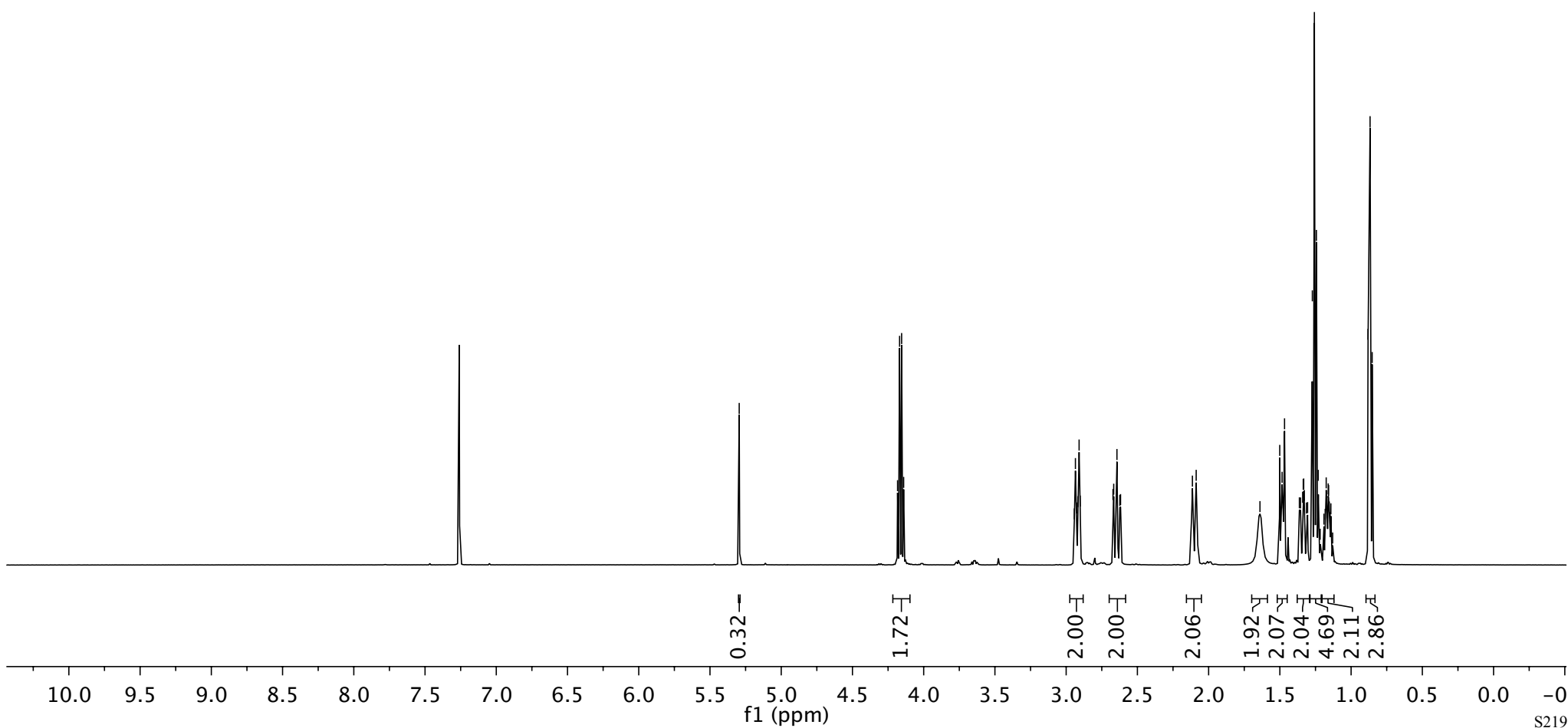


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	32
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.6
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

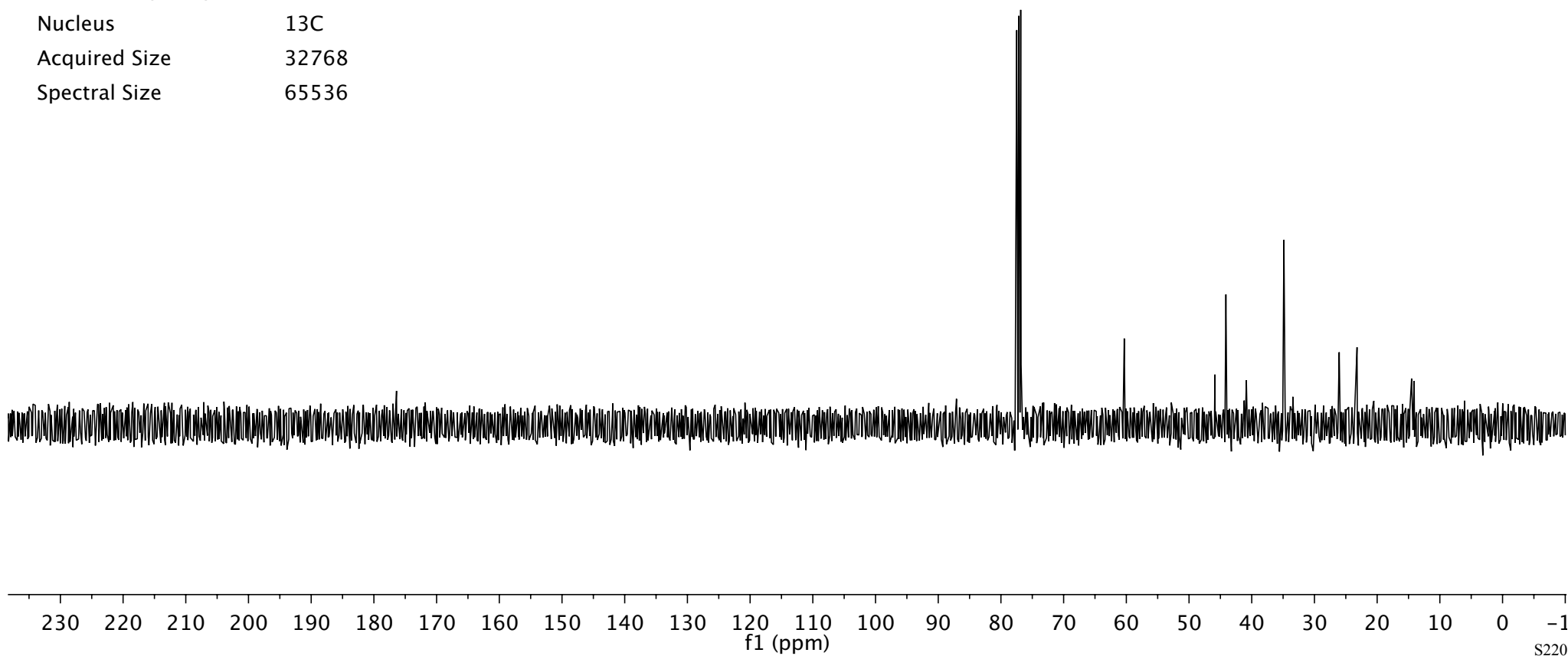
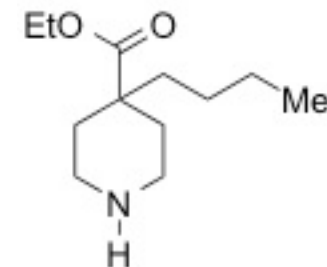


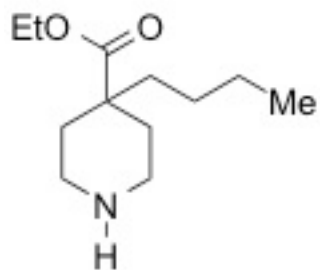


7.26 CDCl₃
 5.29 CH₂Cl₂
 4.18
 4.17
 4.15
 4.14
 2.94
 2.93
 2.93
 2.92
 2.91
 2.90
 2.67
 2.67
 2.64
 2.62
 2.62
 2.11
 2.09
 1.64
 1.50
 1.48
 1.48
 1.47
 1.36
 1.35
 1.34
 1.34
 1.33
 1.33
 1.31
 1.31
 1.27
 1.26
 1.24
 1.23
 1.22
 1.19
 1.18
 1.17
 1.17
 1.16
 1.16
 1.15
 1.15
 1.14
 1.13
 0.88
 0.87
 0.85



Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.3107
Spectrometer Frequency	100.58
Spectral Width	25000.0
Lowest Frequency	-1025.5
Nucleus	13C
Acquired Size	32768
Spectral Size	65536





—176.39

77.48 CDCl₃
77.16 CDCl₃
76.84 CDCl₃

—60.33

~45.87

~44.12

~40.87

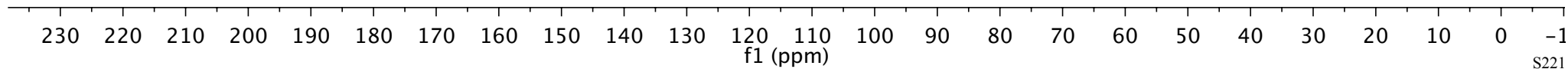
~34.87

~26.05

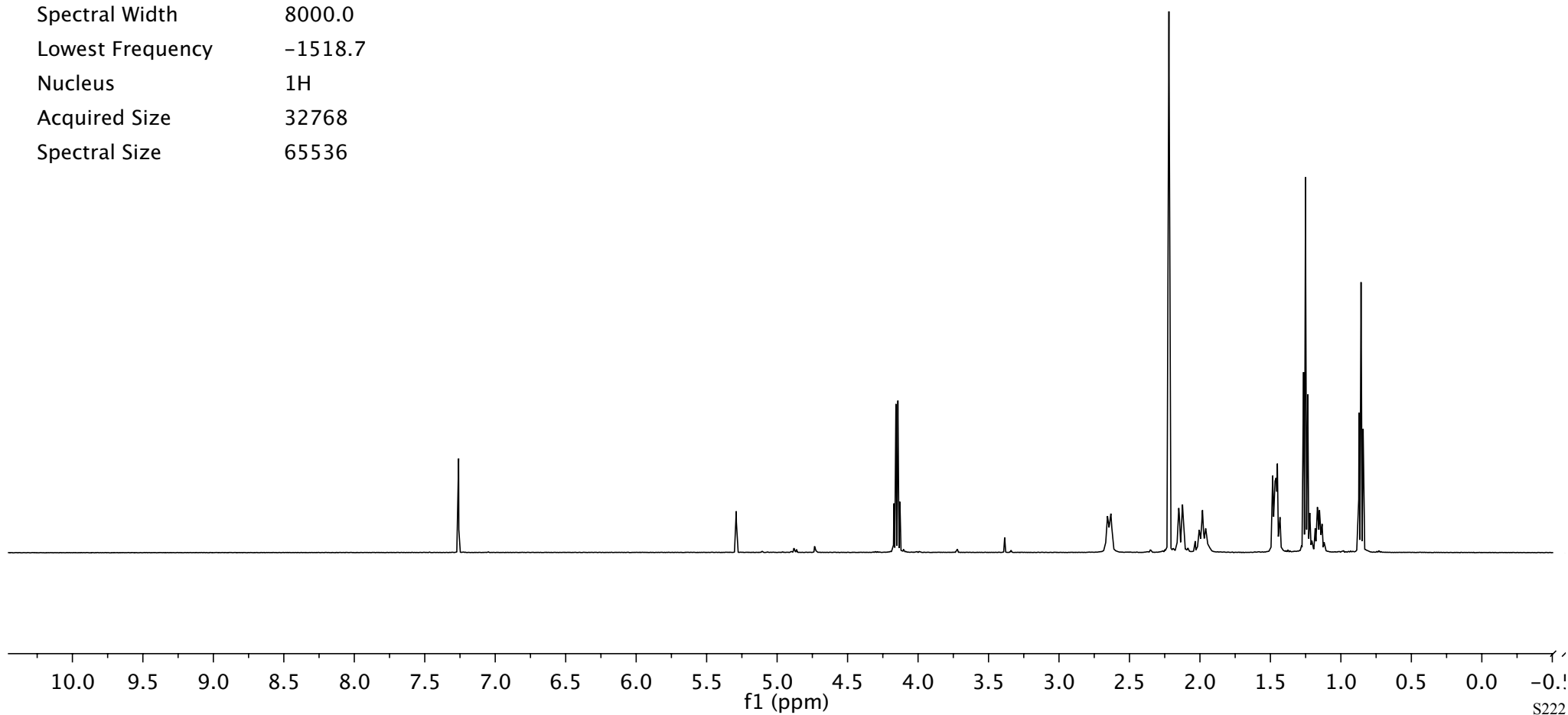
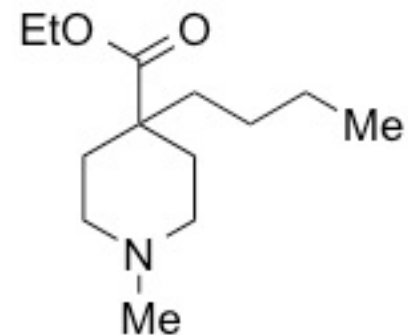
~23.21

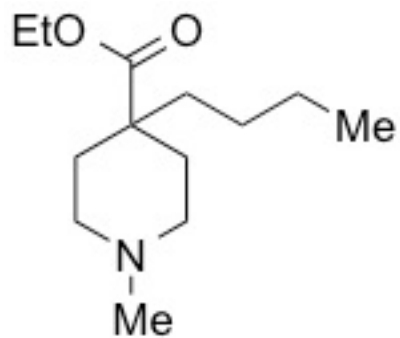
~14.51

~14.08



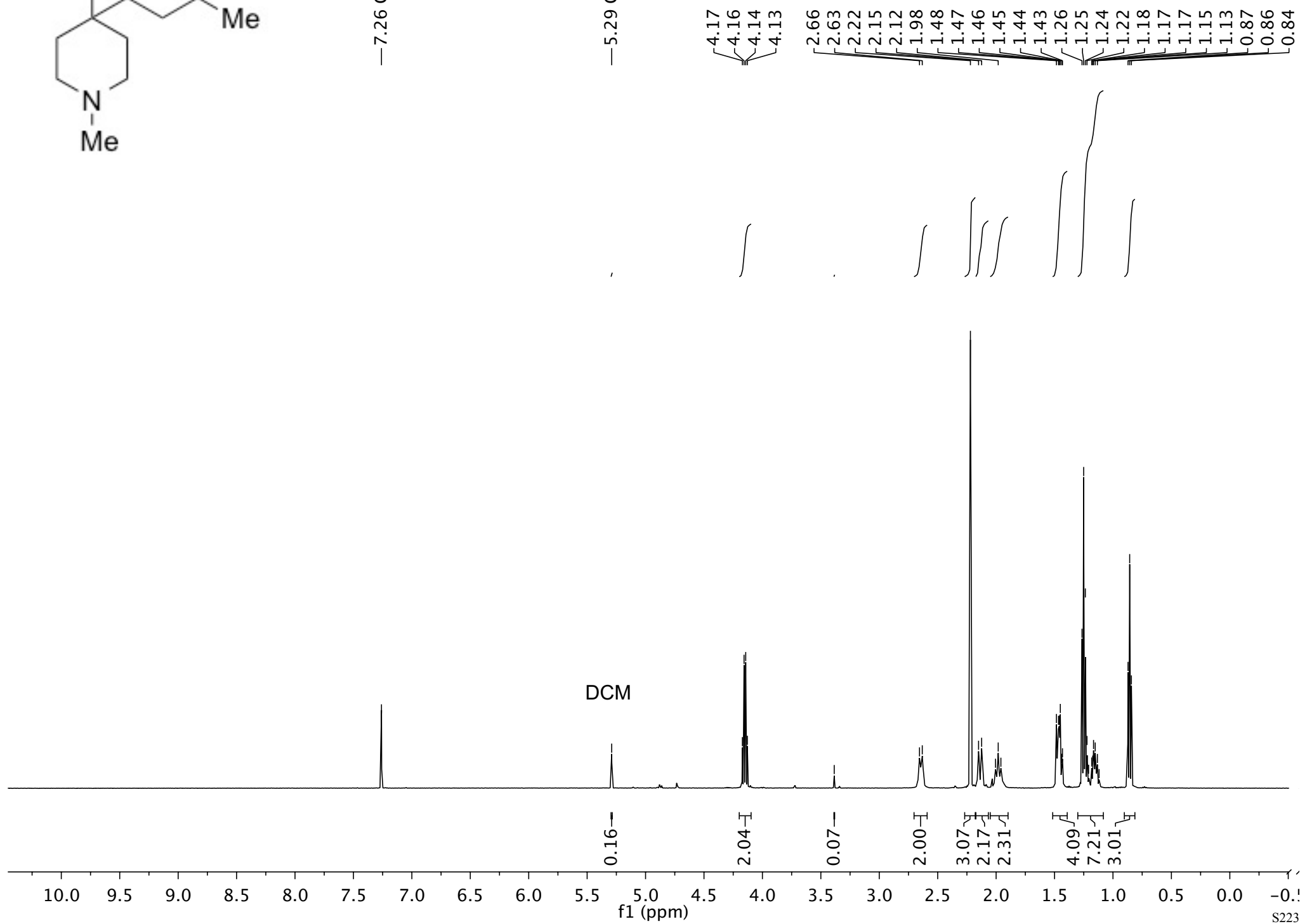
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	19.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	54
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	499.43
Spectral Width	8000.0
Lowest Frequency	-1518.7
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



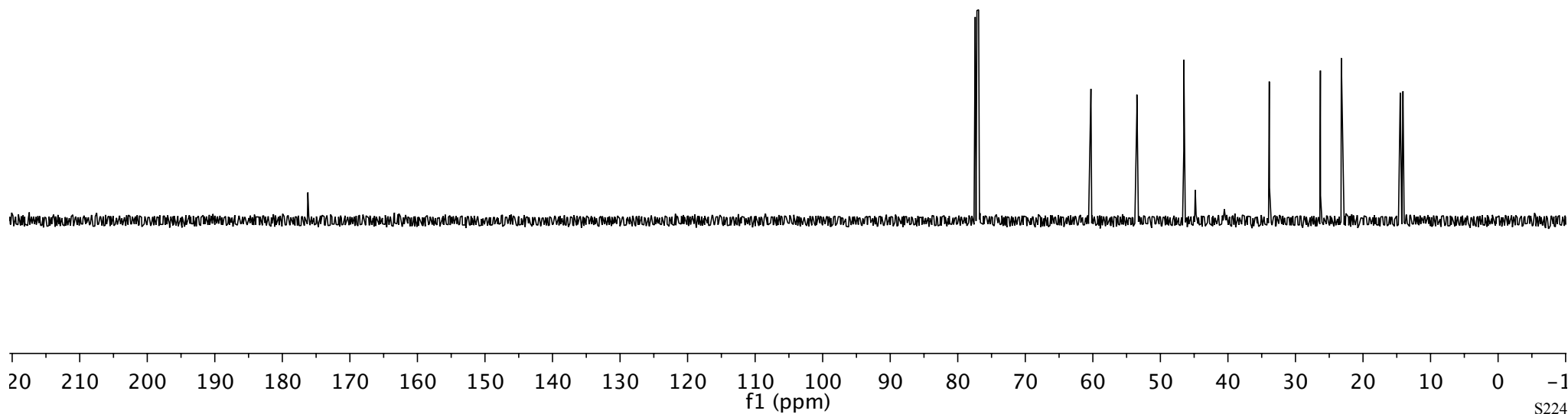
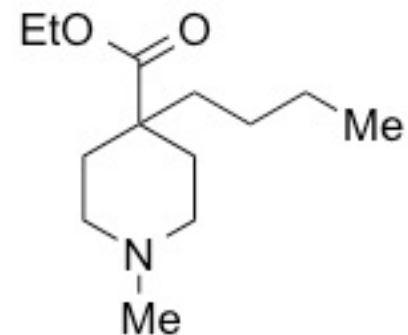


—7.26 CDCl₃

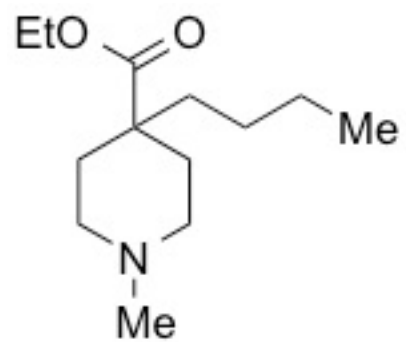
—5.29 CH₂Cl₂



Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1272.5
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



—176.22

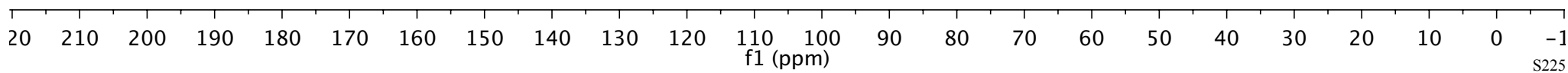


77.41 CDCl₃
77.16 CDCl₃
76.91 CDCl₃

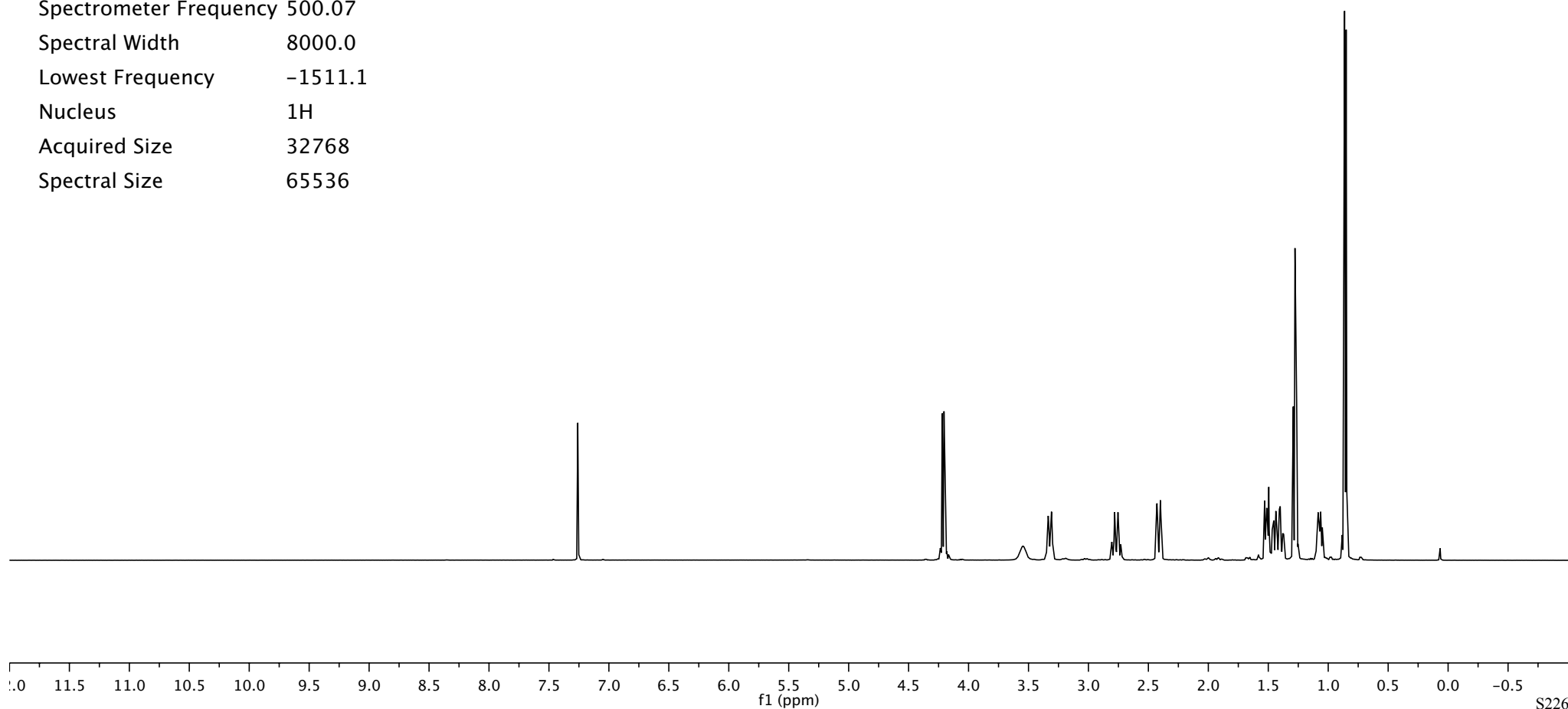
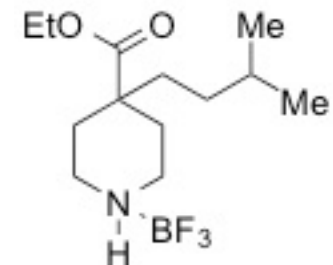
60.28
53.48
46.53
44.84
40.53
33.87

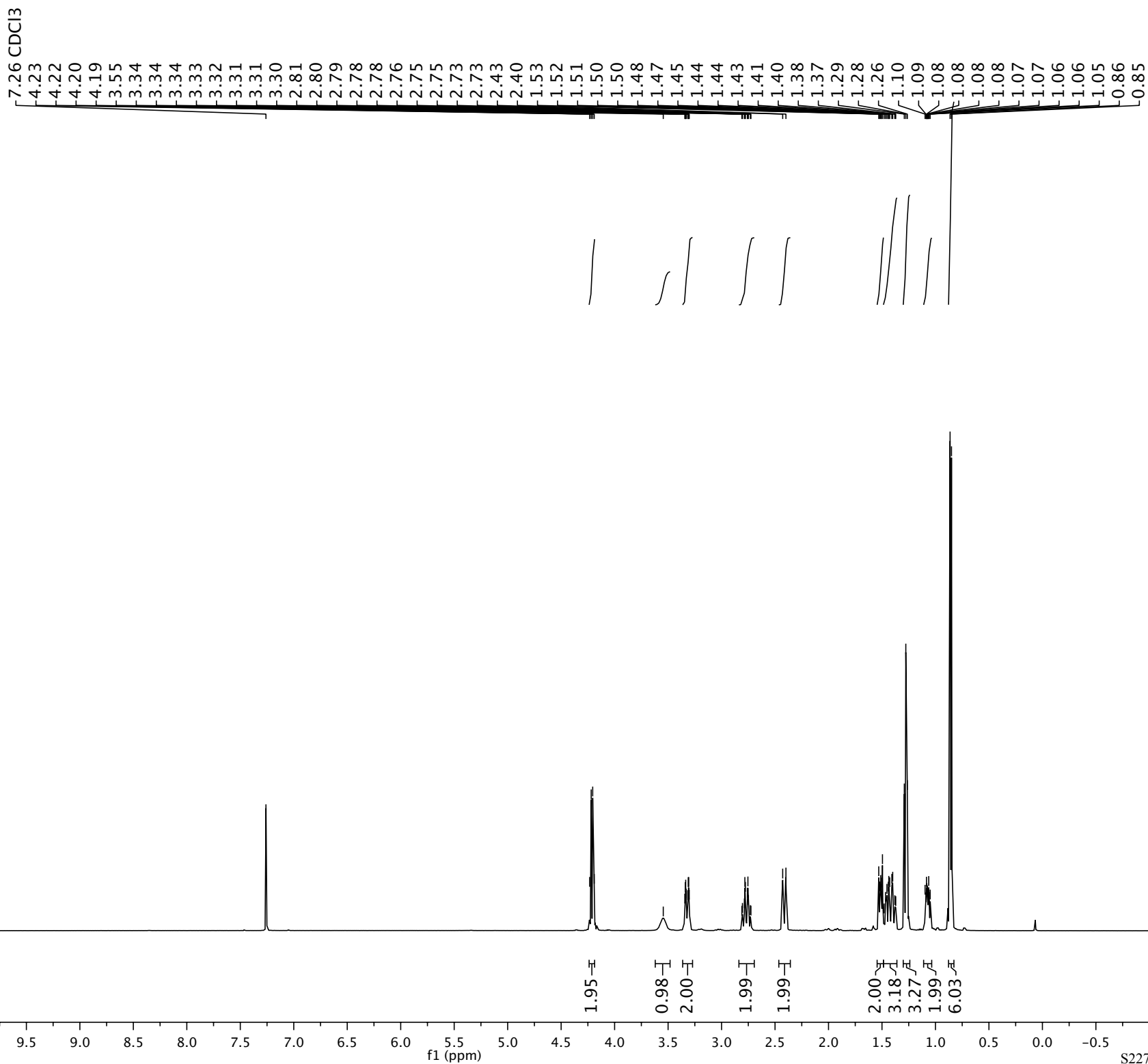
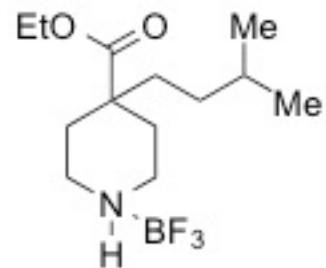
26.31
23.21

14.48
14.08

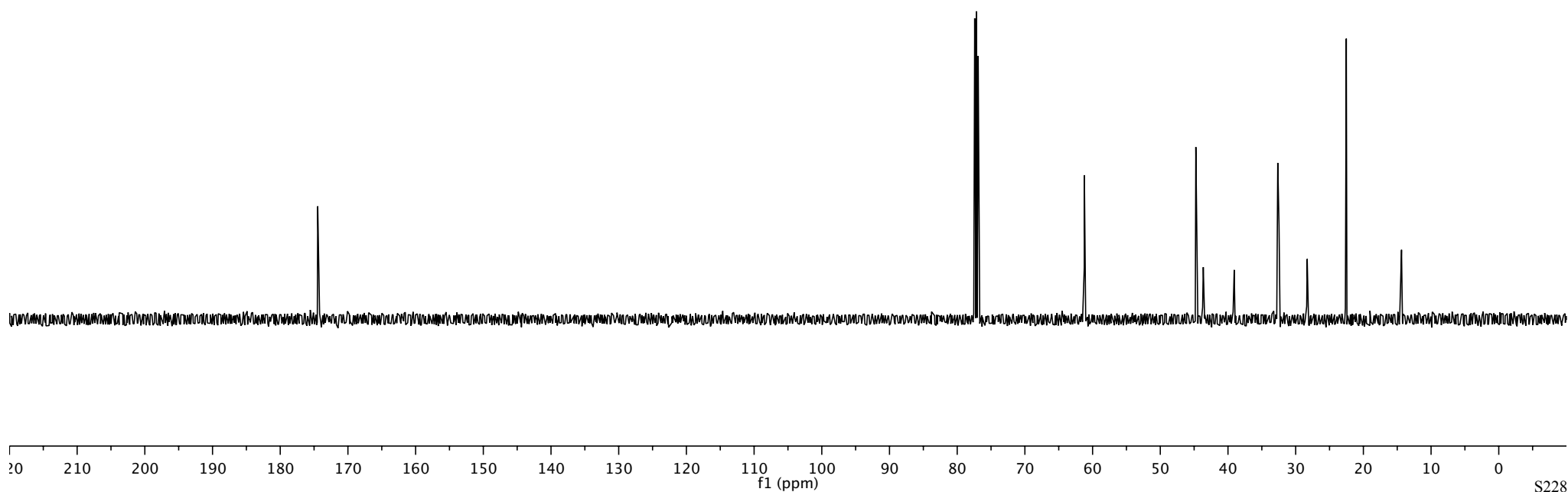
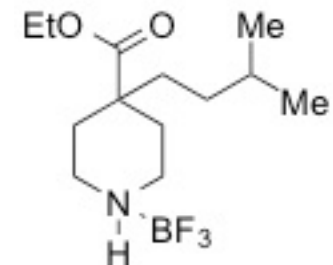


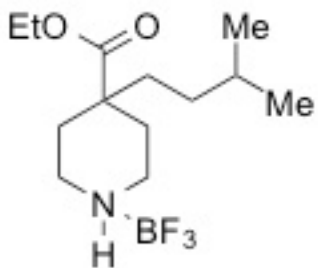
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	32
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1511.1
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536





Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Number of Scans	520
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2200.0
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536





—174.46

—77.16 CDCl₃

—61.21

—44.75

—43.65

—39.09

—32.65

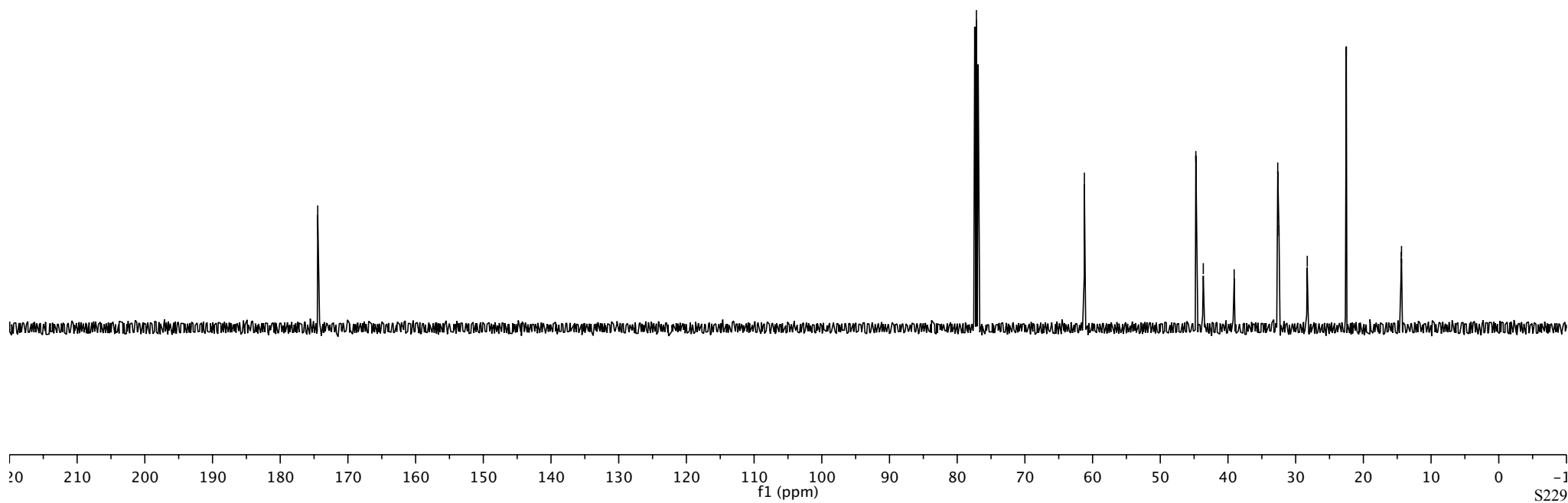
—32.47

—28.29

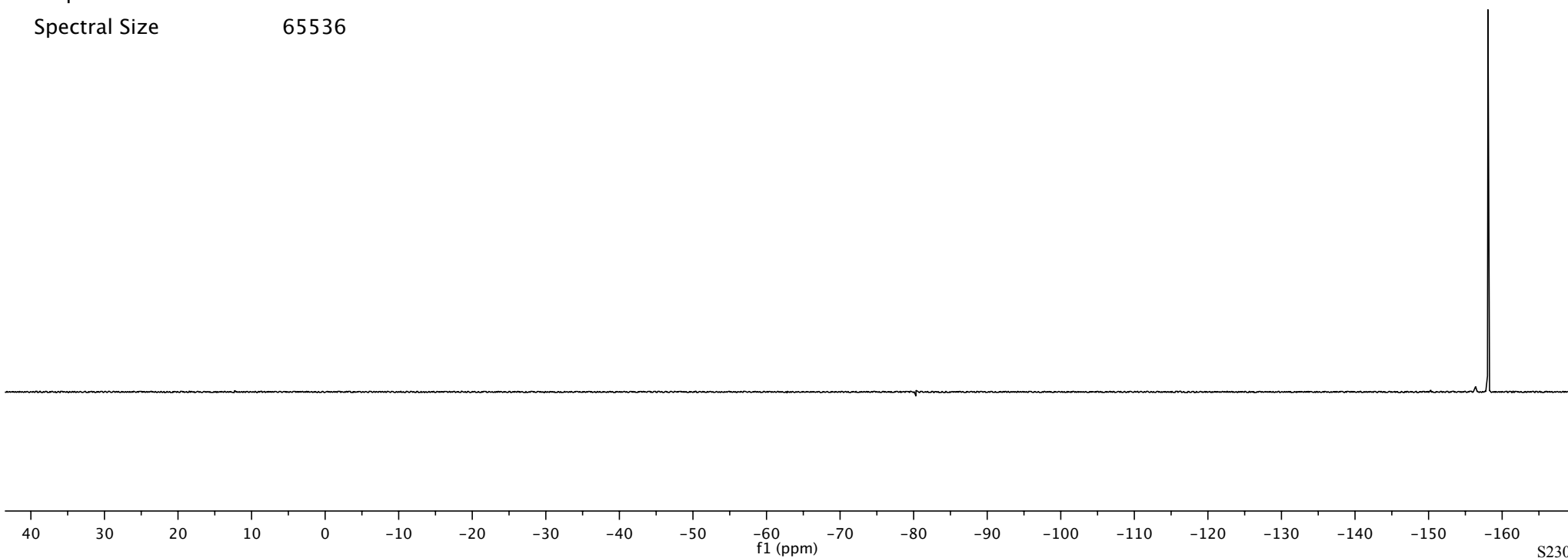
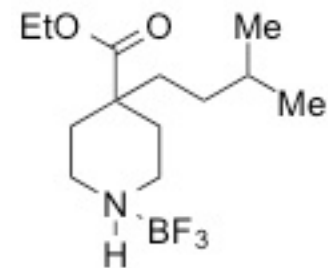
—22.53

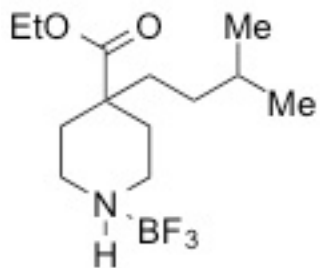
—14.41

—14.37

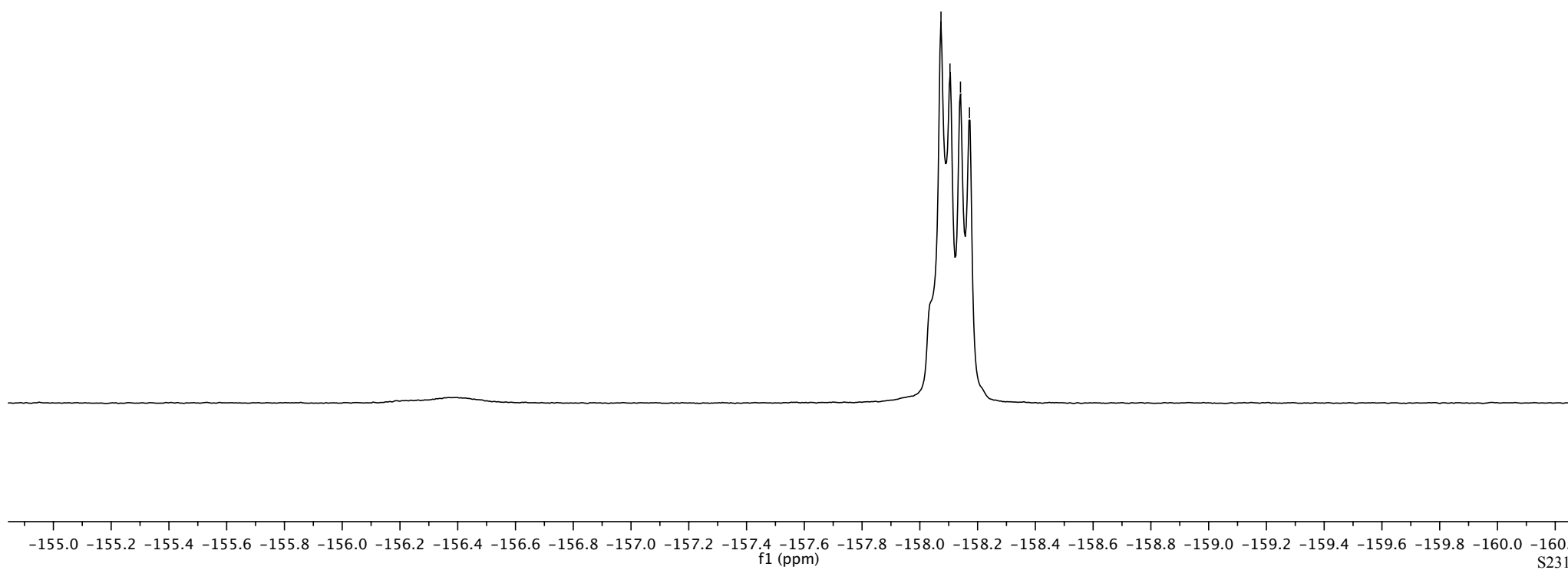


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	120
Receiver Gain	48
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency	-79531.9
Nucleus	¹⁹ F
Acquired Size	32768
Spectral Size	65536

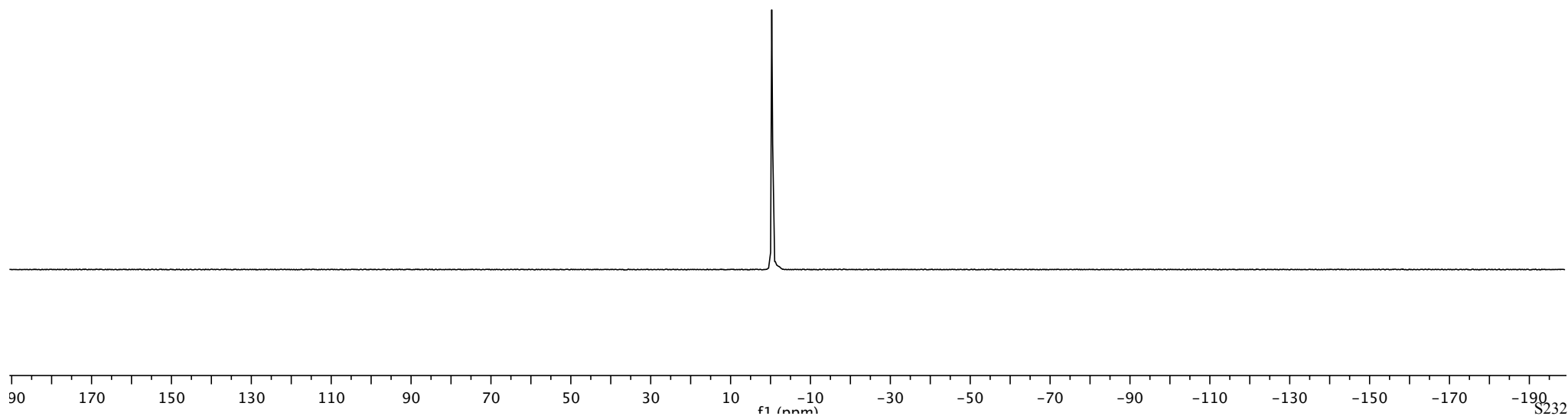
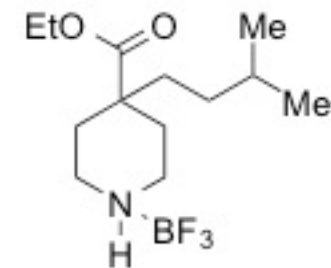


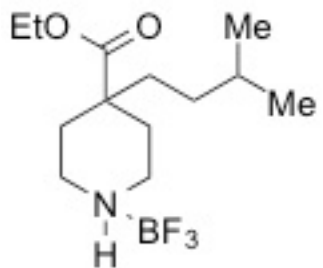


-158.07
-158.10
-158.14
-158.17

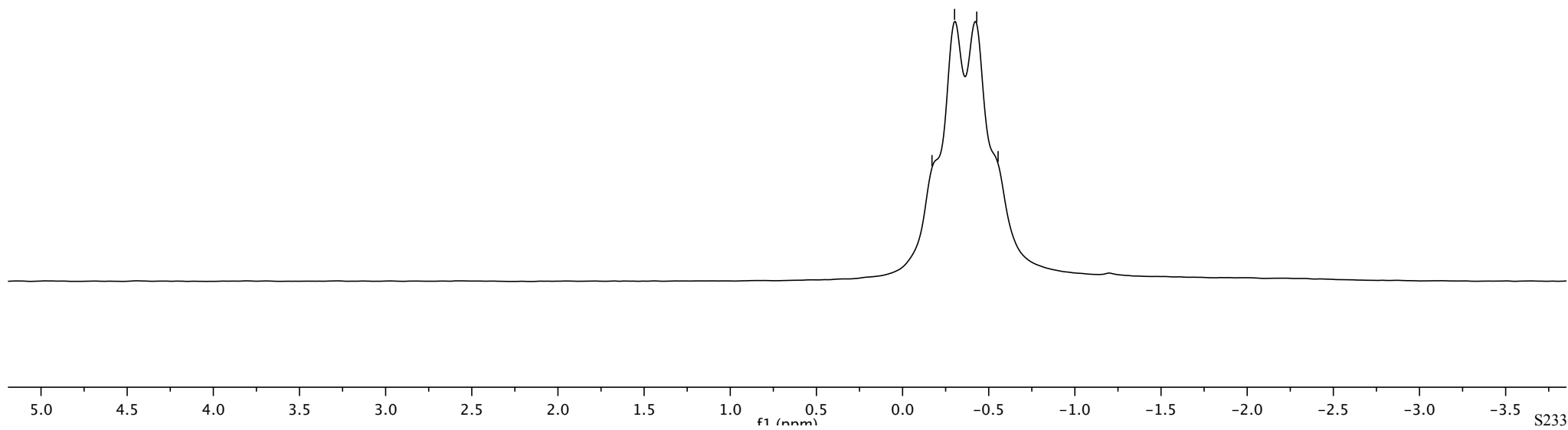


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quadbp
Number of Scans	16
Receiver Gain	58
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.6554
Spectrometer Frequency	128.25
Spectral Width	50000.0
Lowest Frequency	-25560.0
Nucleus	11B
Acquired Size	32768
Spectral Size	65536

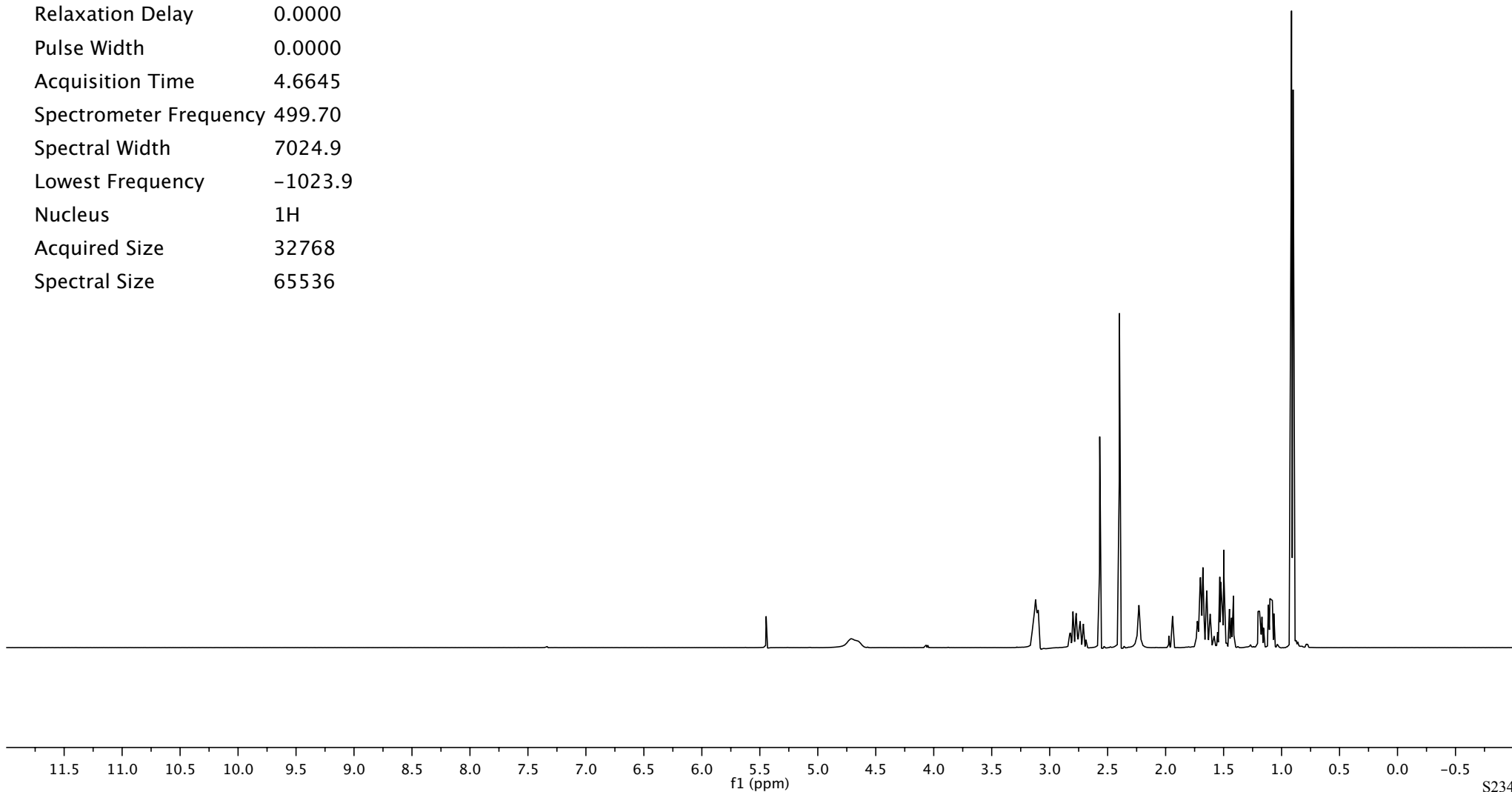
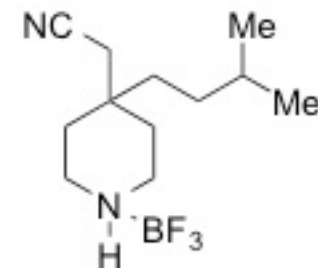


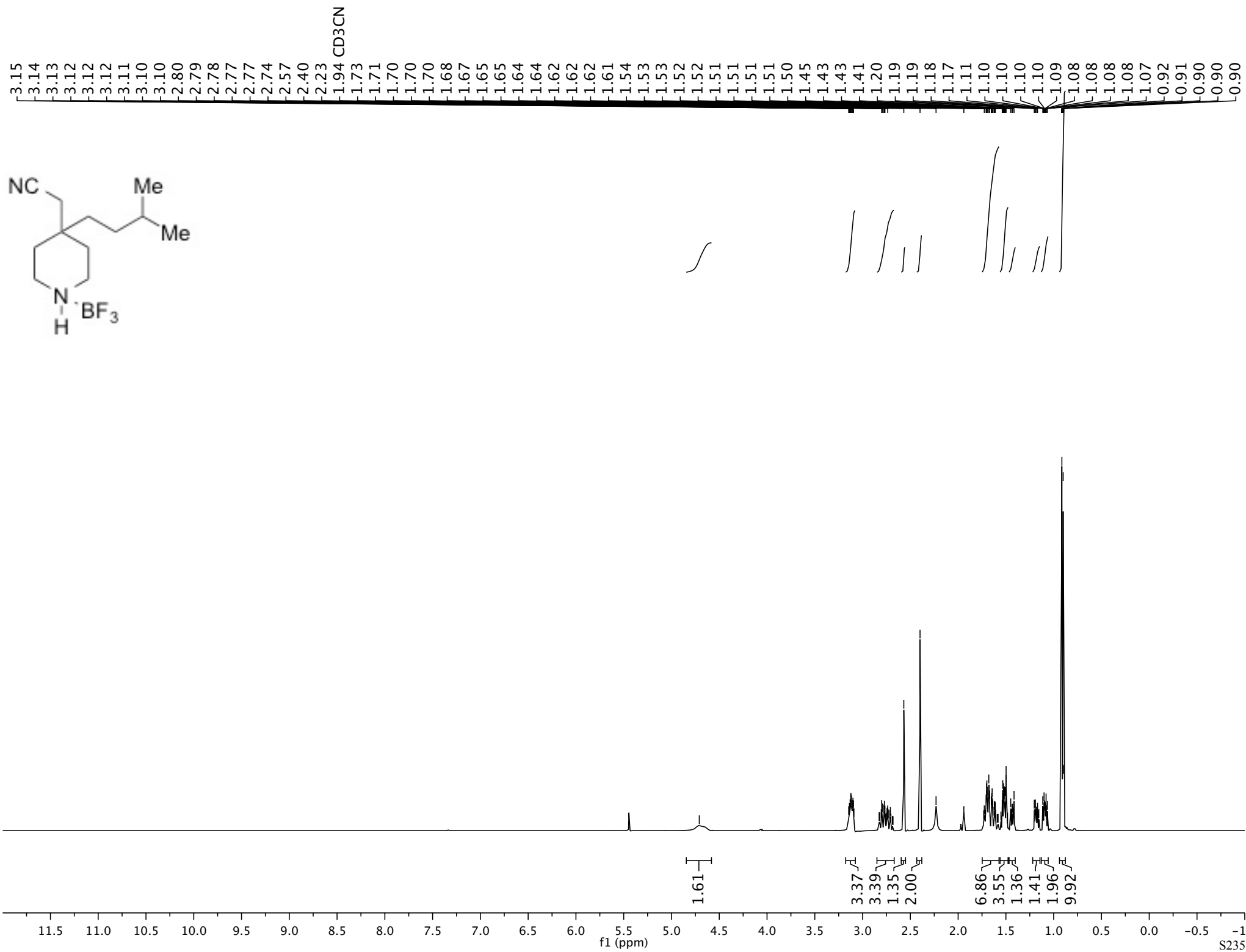


--0.17
--0.30
--0.43
--0.55

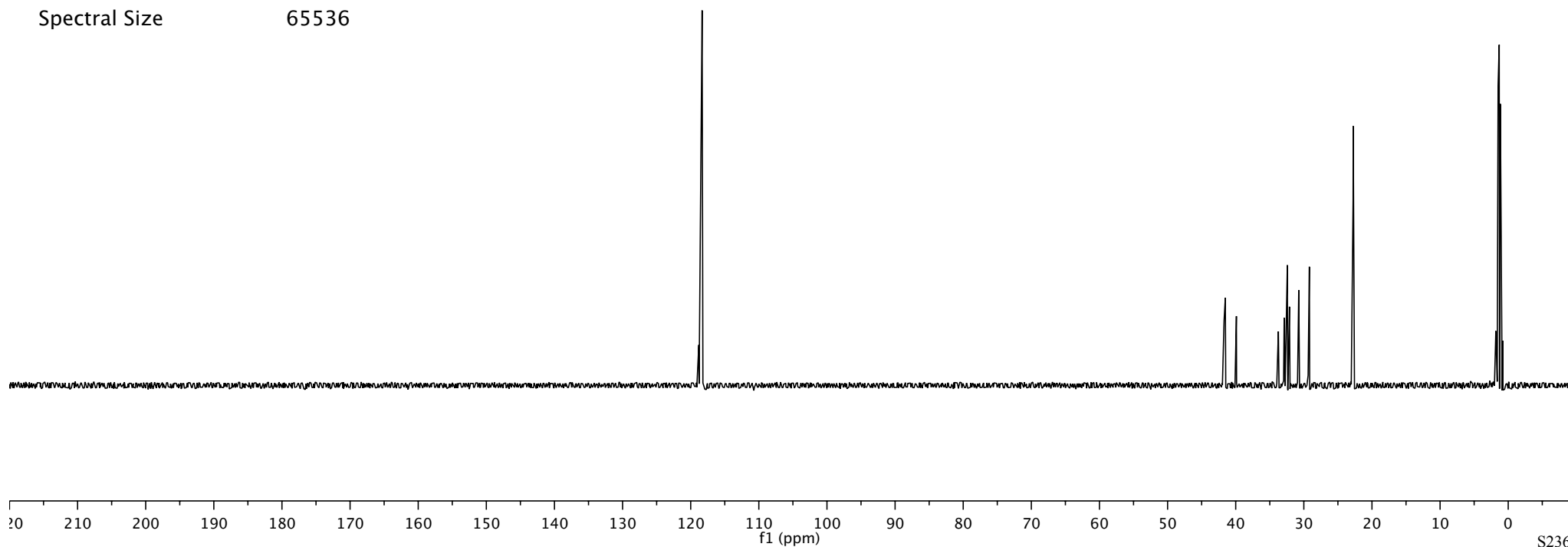
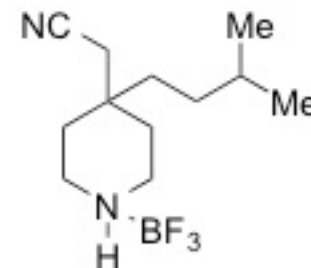


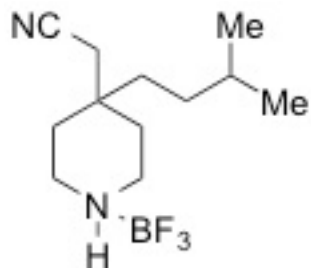
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CD3CN
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	8
Receiver Gain	36
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.70
Spectral Width	7024.9
Lowest Frequency	-1023.9
Nucleus	^1H
Acquired Size	32768
Spectral Size	65536





Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CD3CN
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	224
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1168.4
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

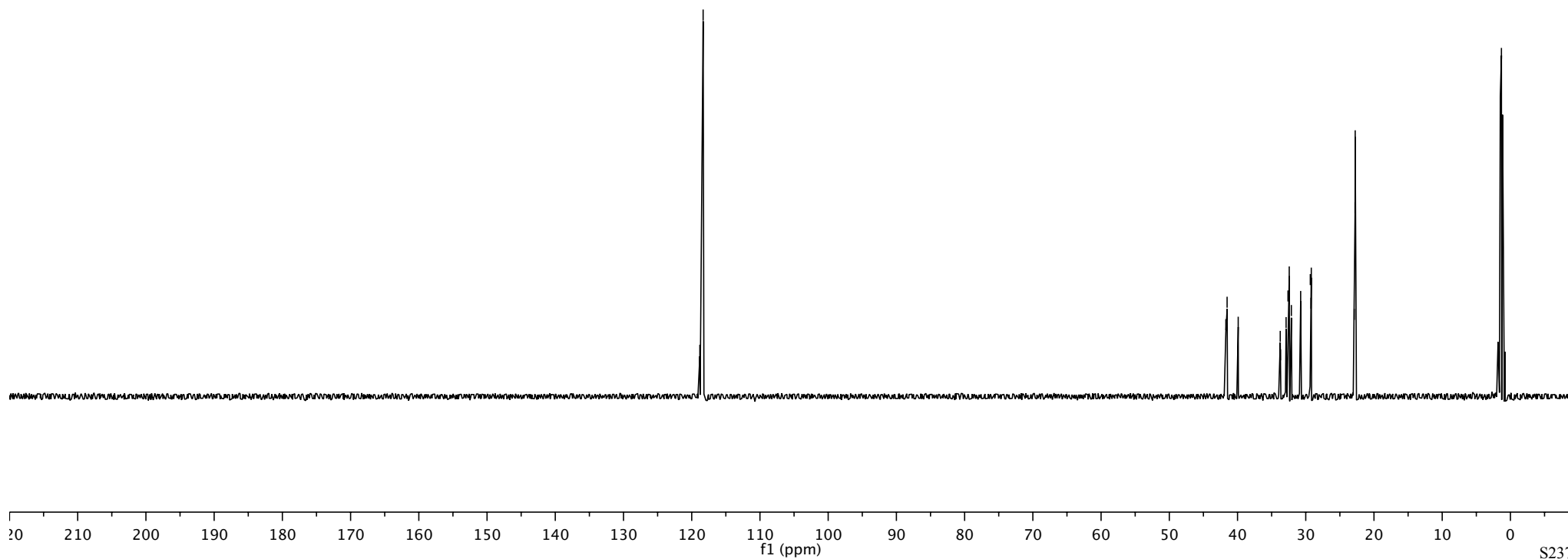




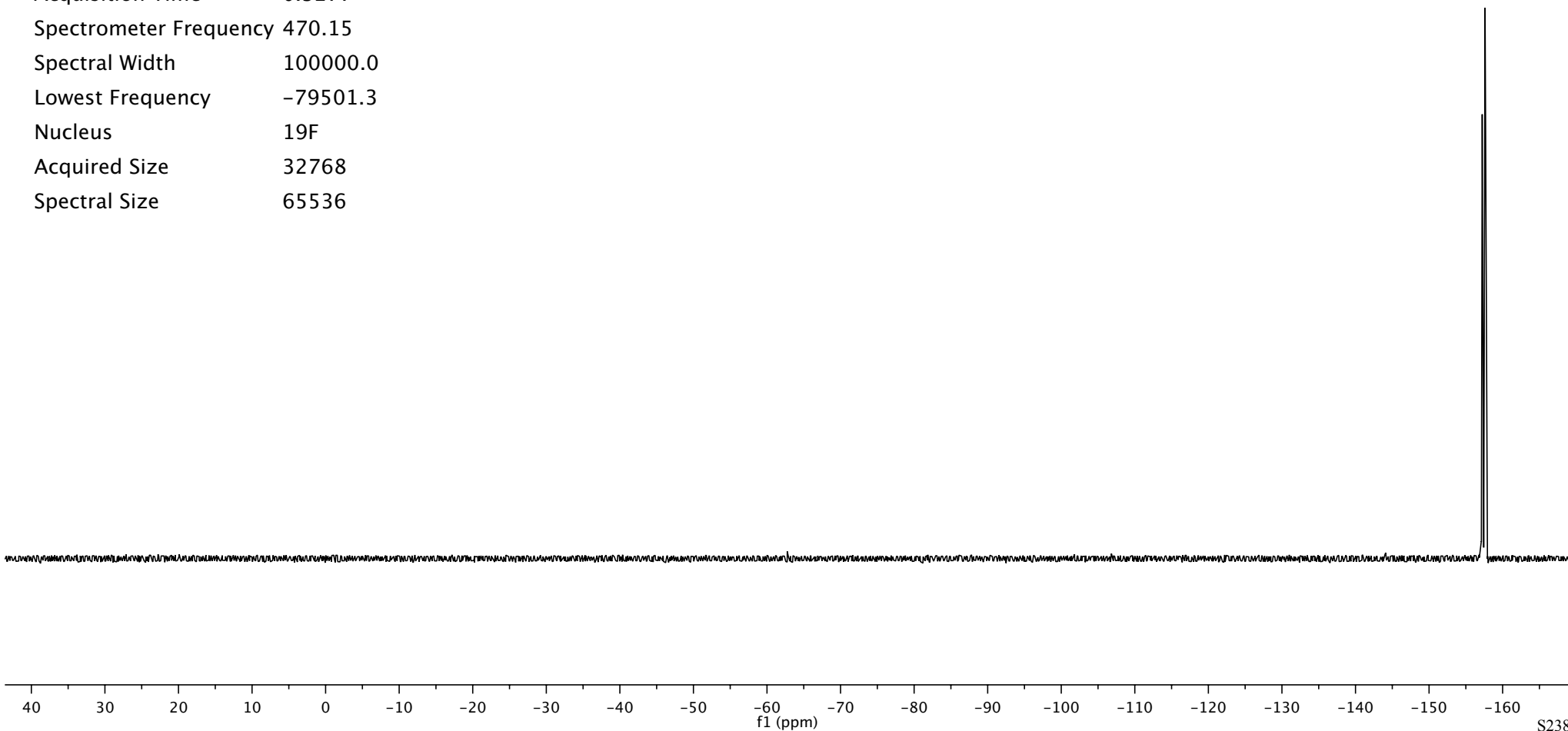
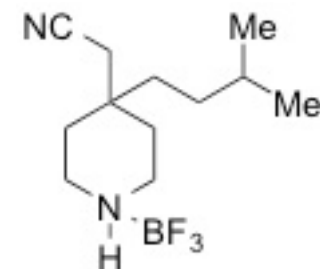
118.87
118.81
118.33

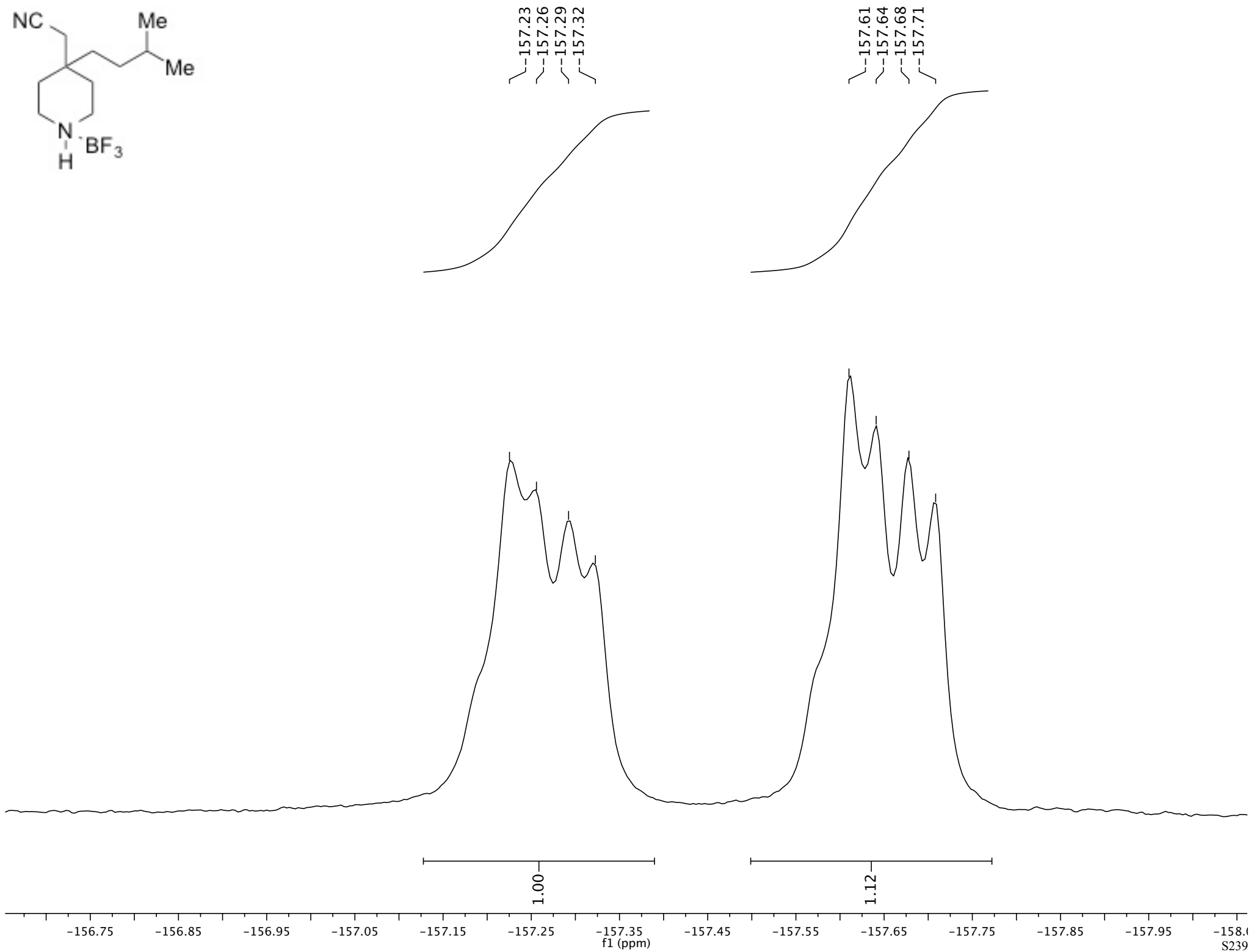
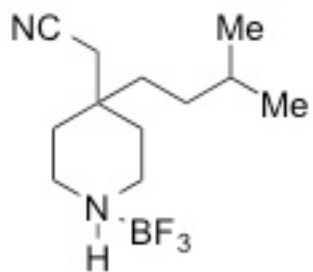
41.71
41.53
39.90
33.74
33.70
32.88
32.60
32.42
32.11
30.75
29.33
29.23
29.19
22.89
22.77
22.75

— 1.32 CD3CN

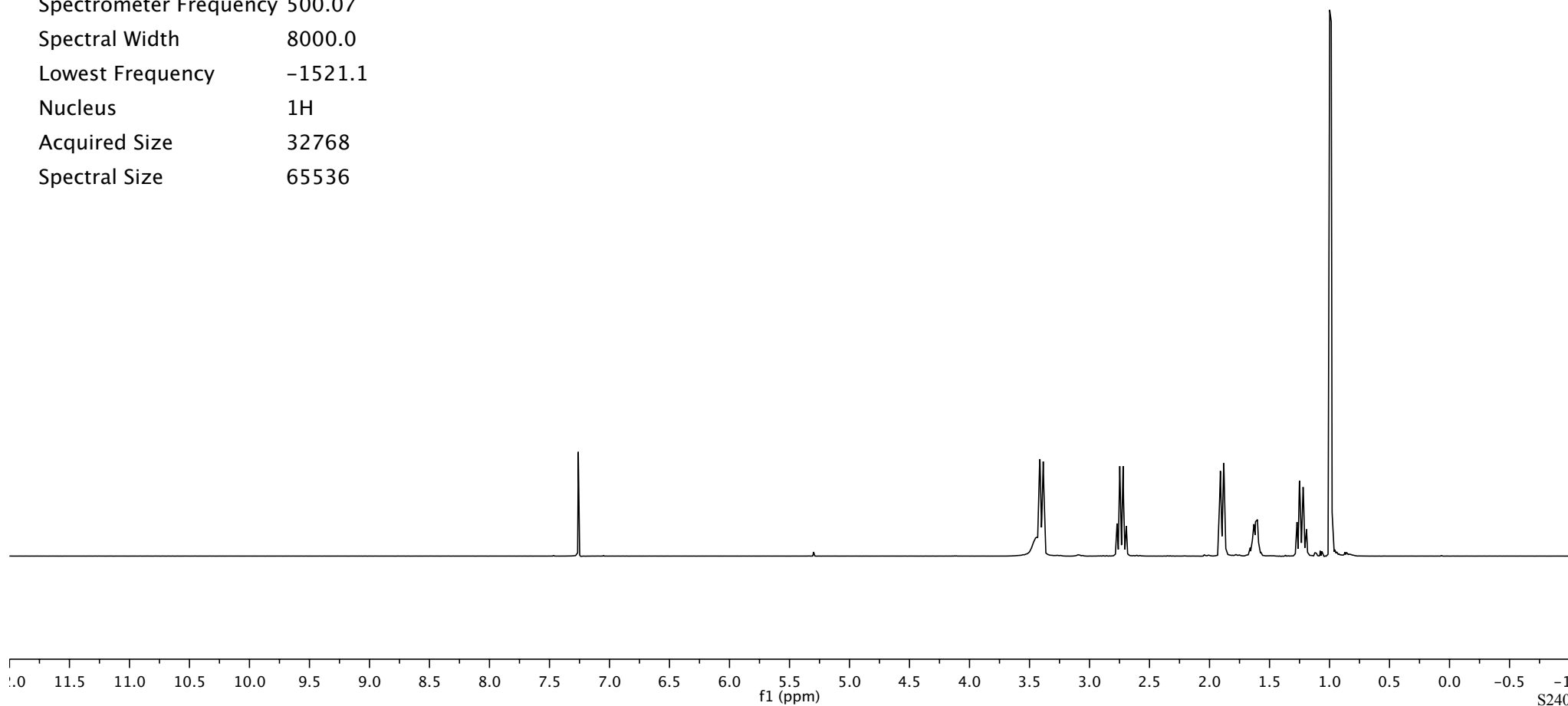
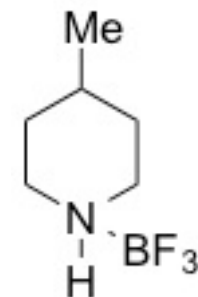


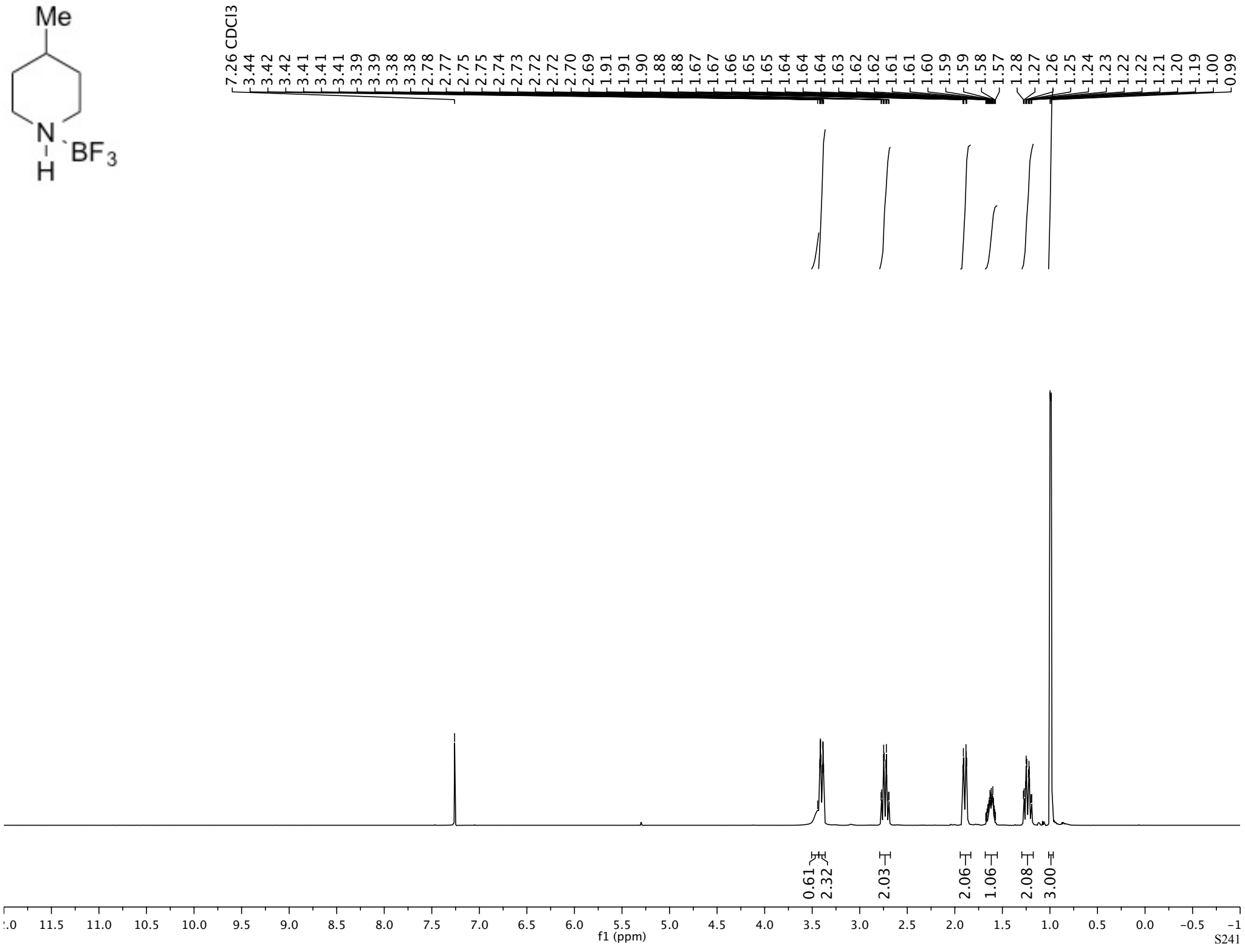
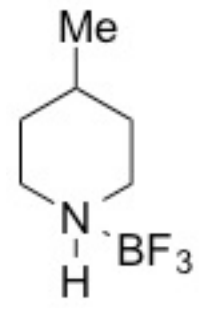
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	64
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency	-79501.3
Nucleus	¹⁹ F
Acquired Size	32768
Spectral Size	65536



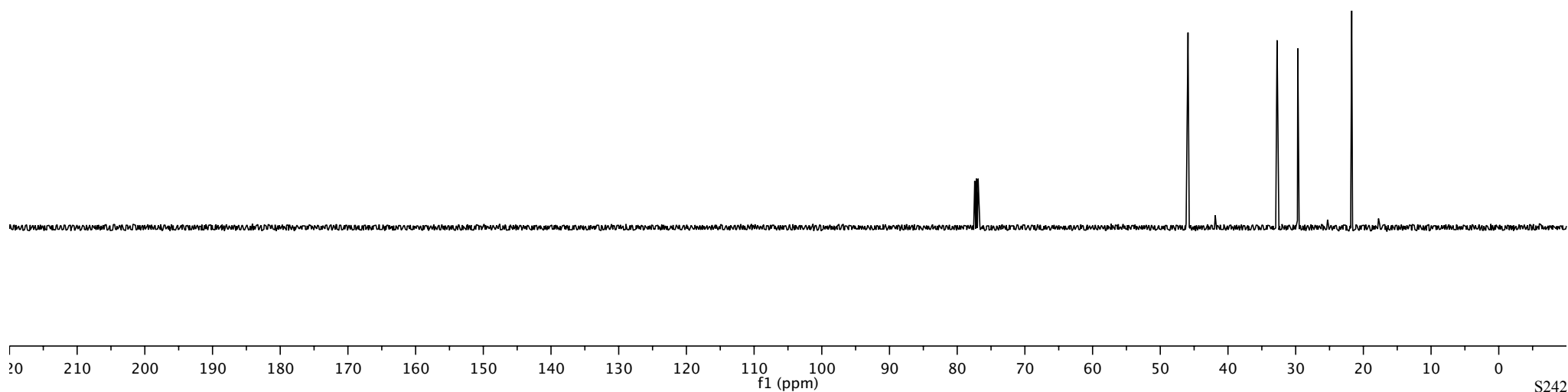
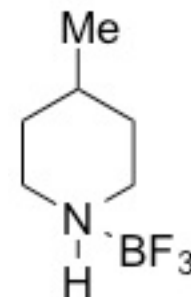


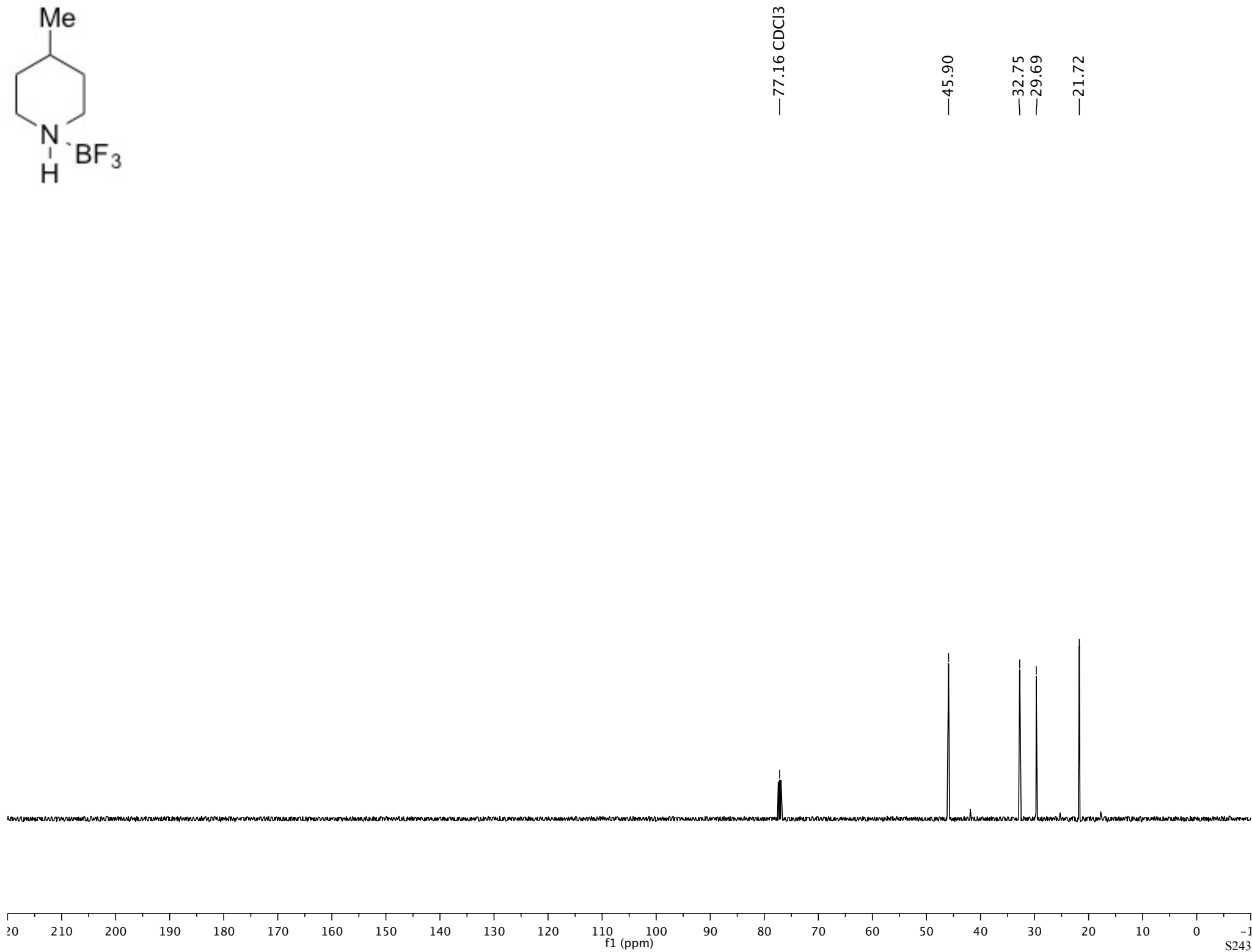
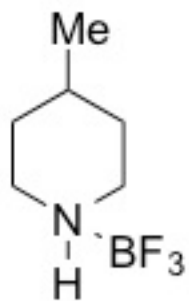
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	32
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



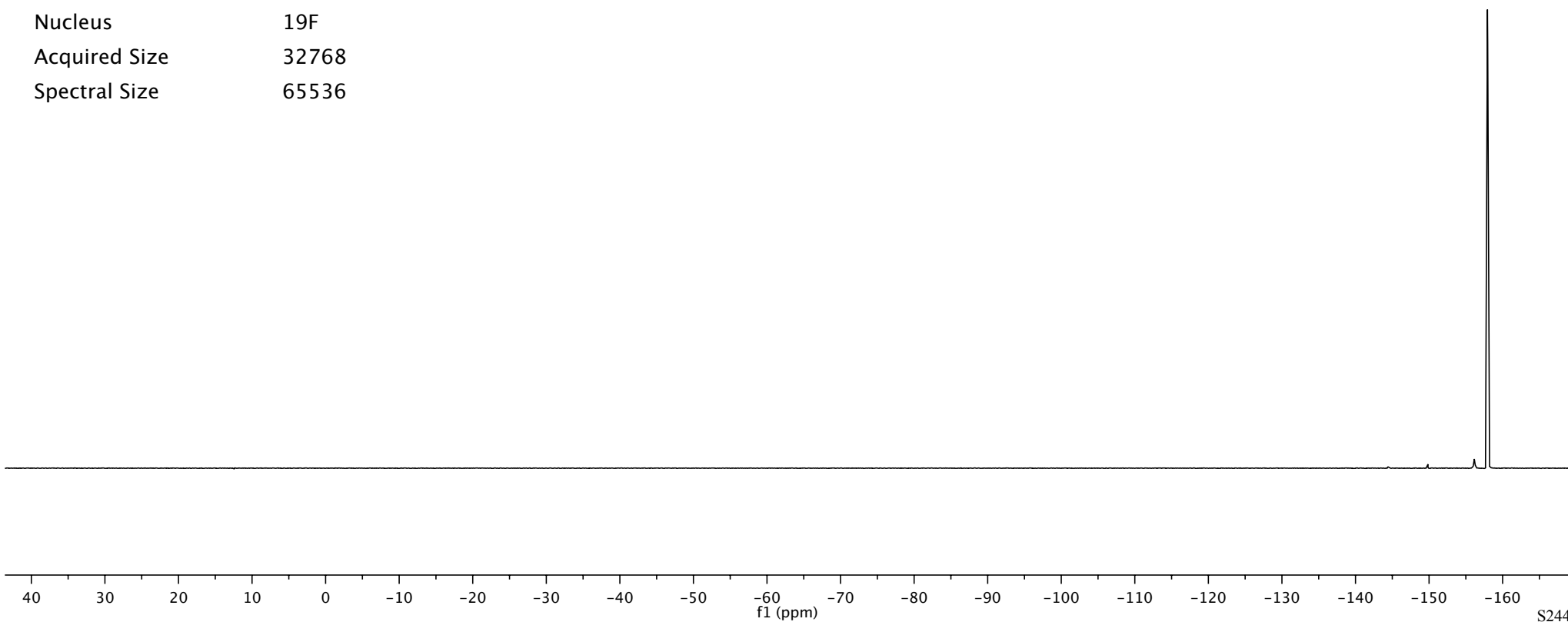
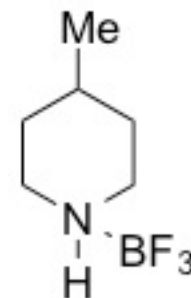


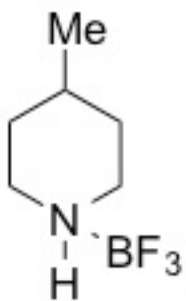
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	64
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1276.5
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



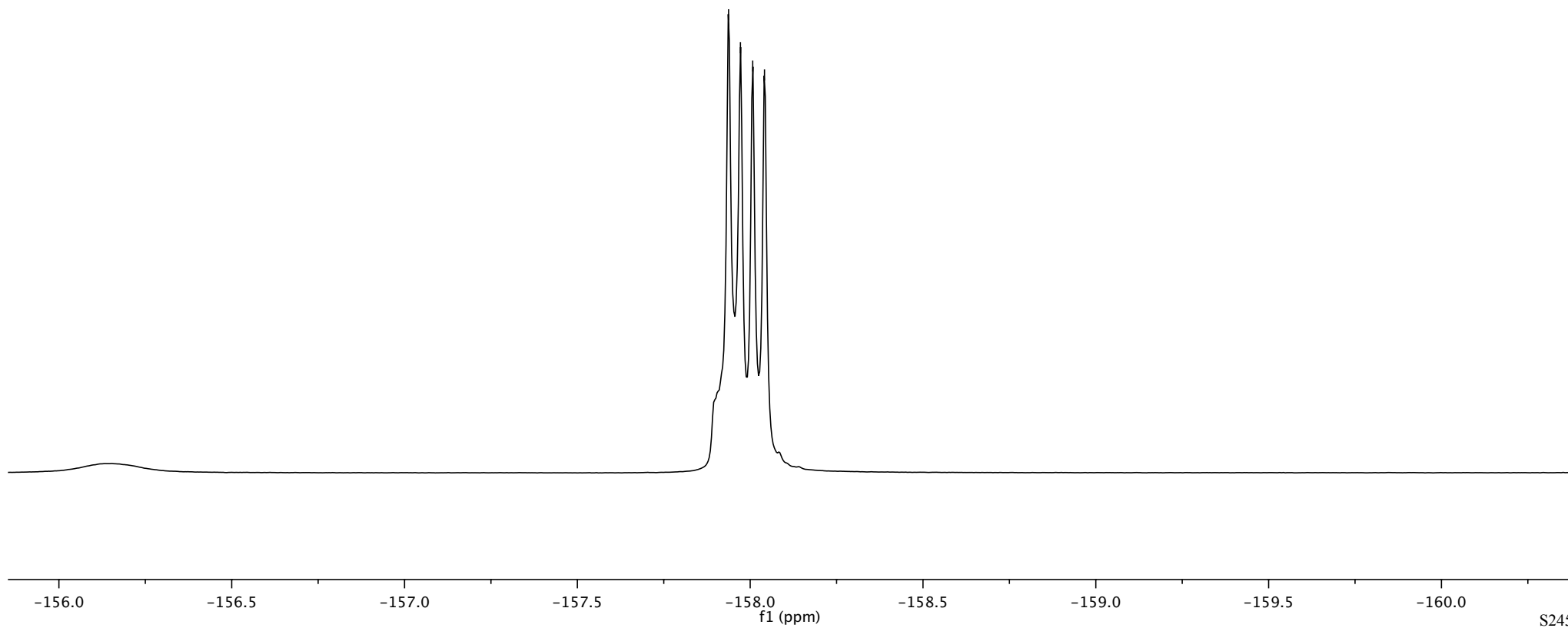


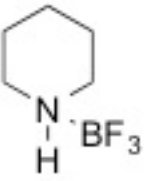
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	64
Receiver Gain	52
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency	-79501.3
Nucleus	19F
Acquired Size	32768
Spectral Size	65536



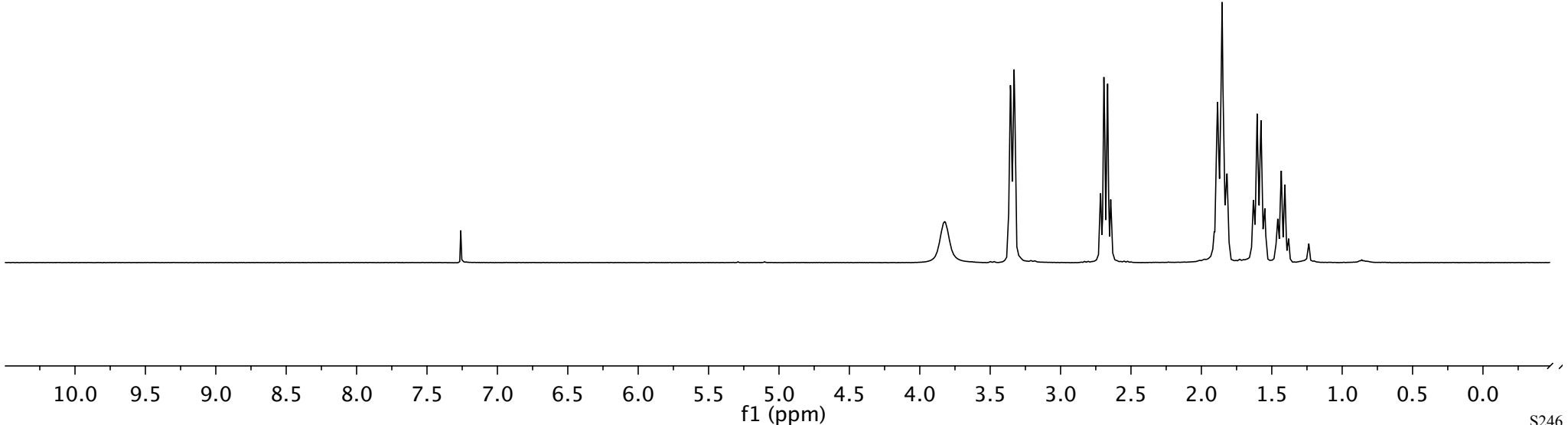


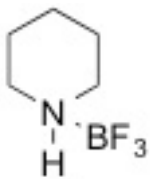
157.94
157.97
158.01
158.04



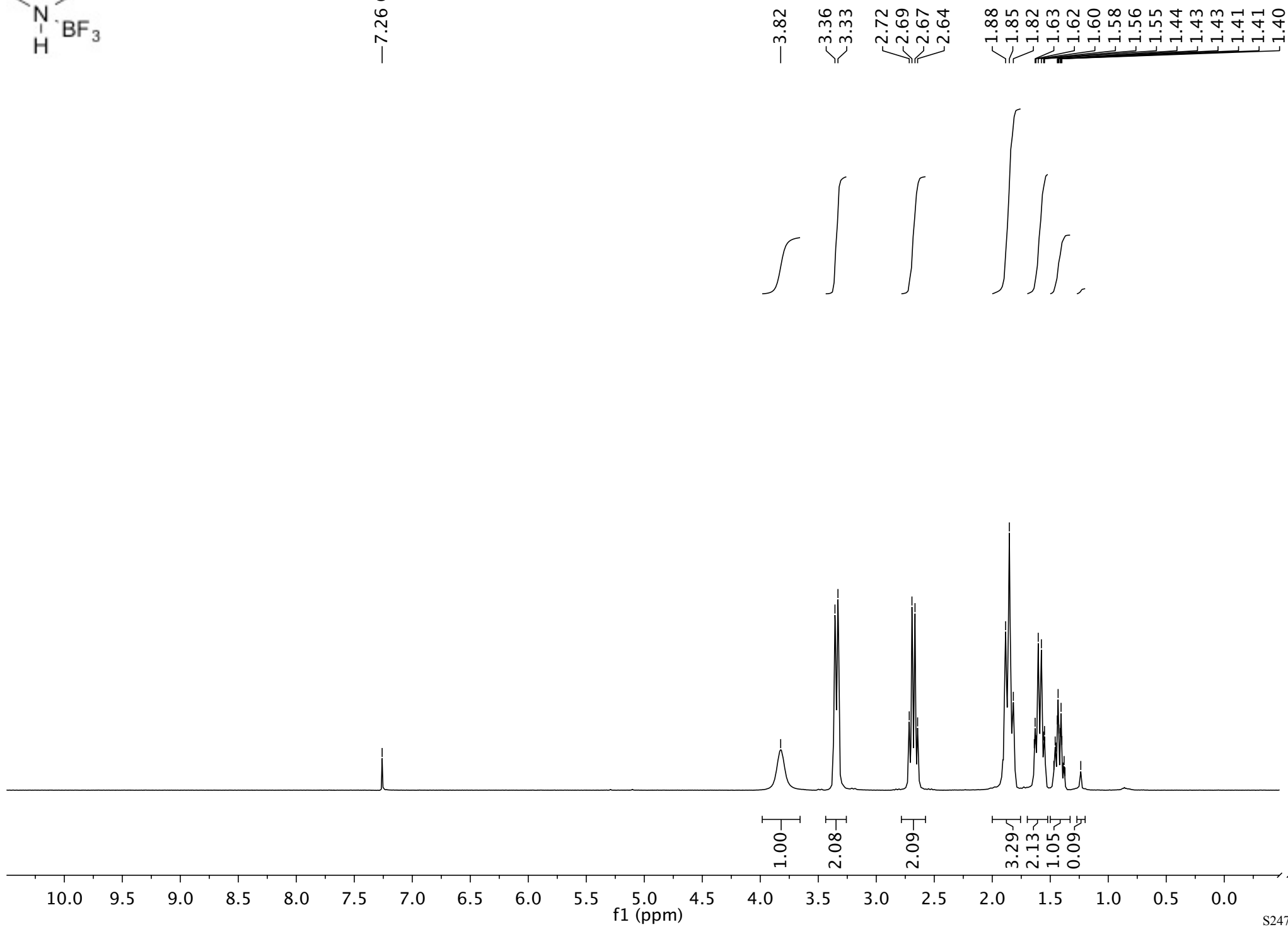


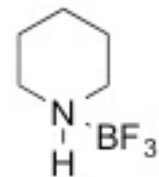
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	44
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	499.43
Spectral Width	8000.0
Lowest Frequency	-1518.4
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



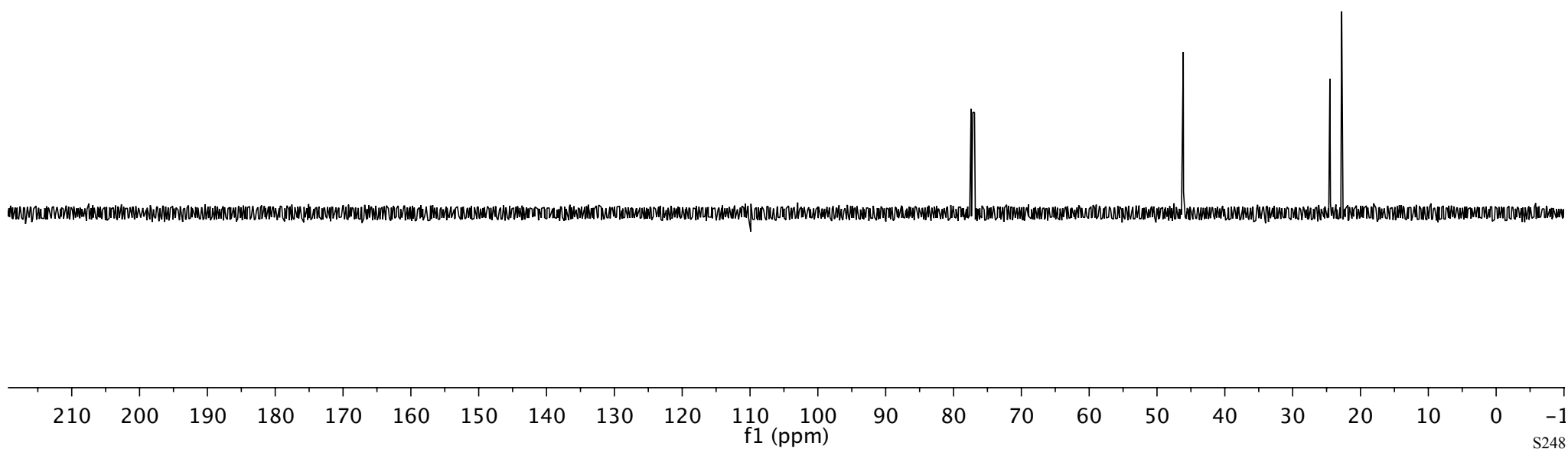


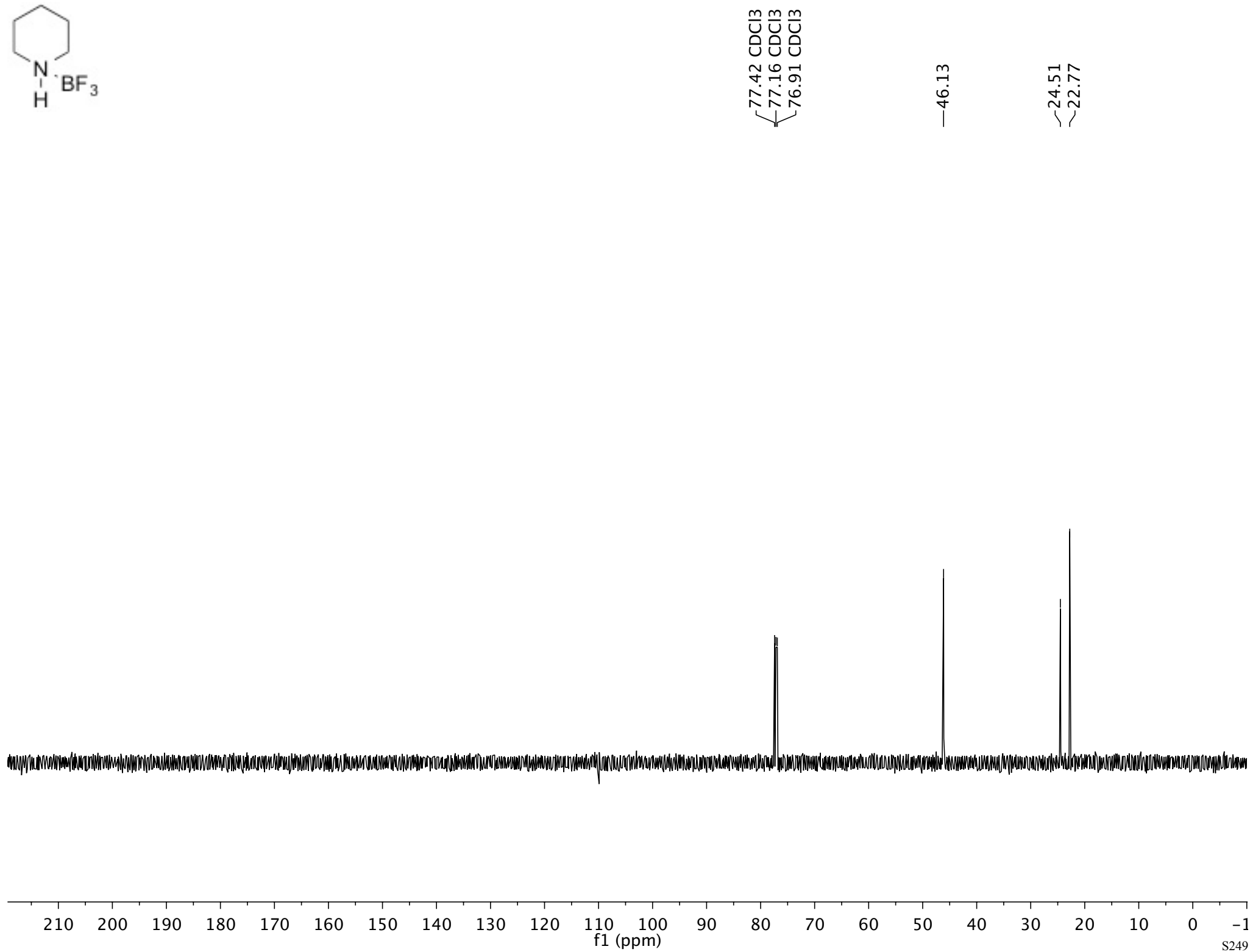
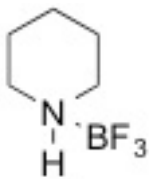
—7.26 CDCl₃

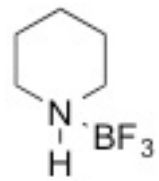




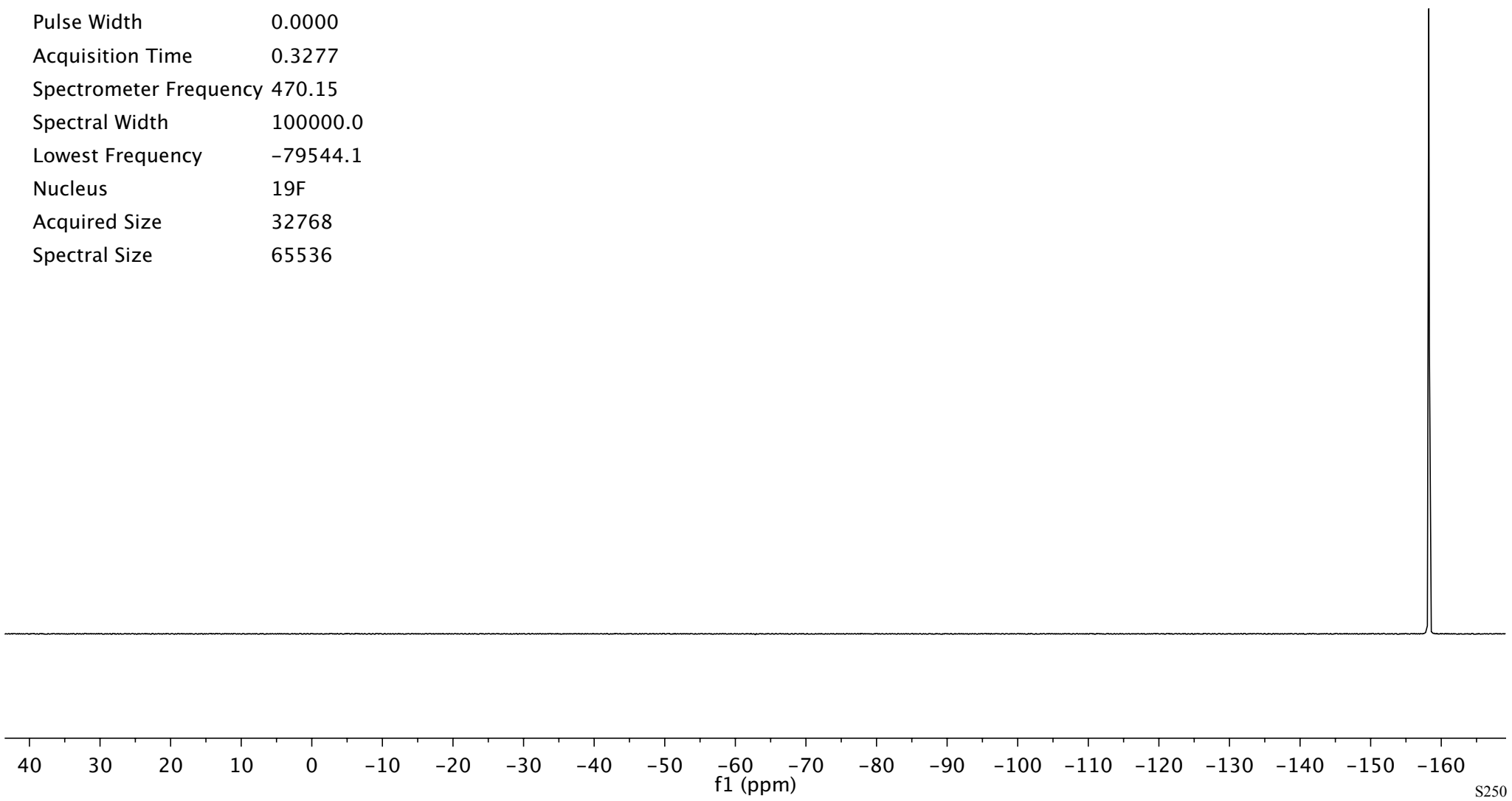
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1274.6
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

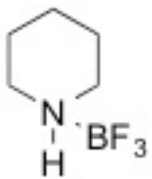




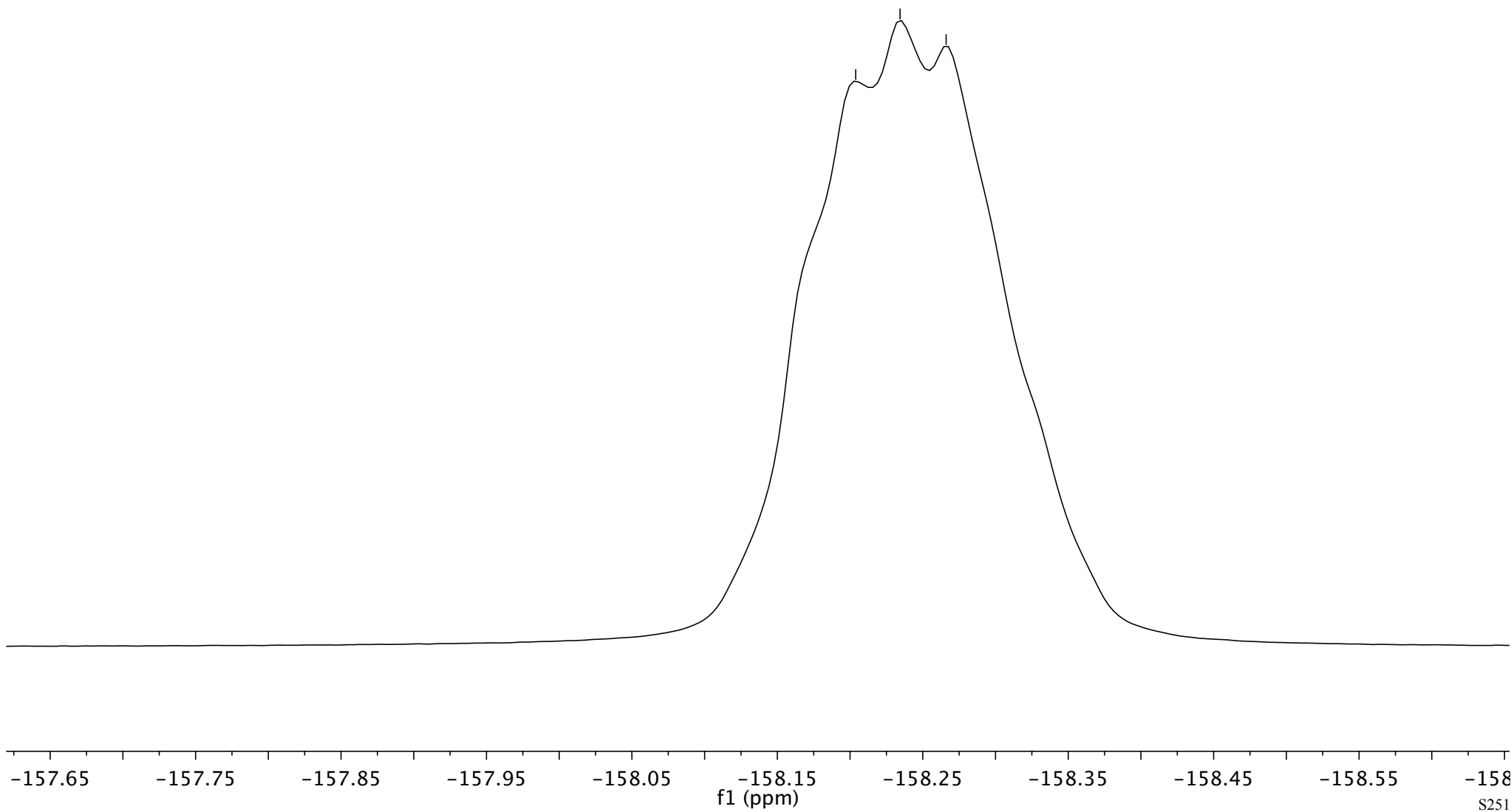


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	50
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency	-79544.1
Nucleus	19F
Acquired Size	32768
Spectral Size	65536

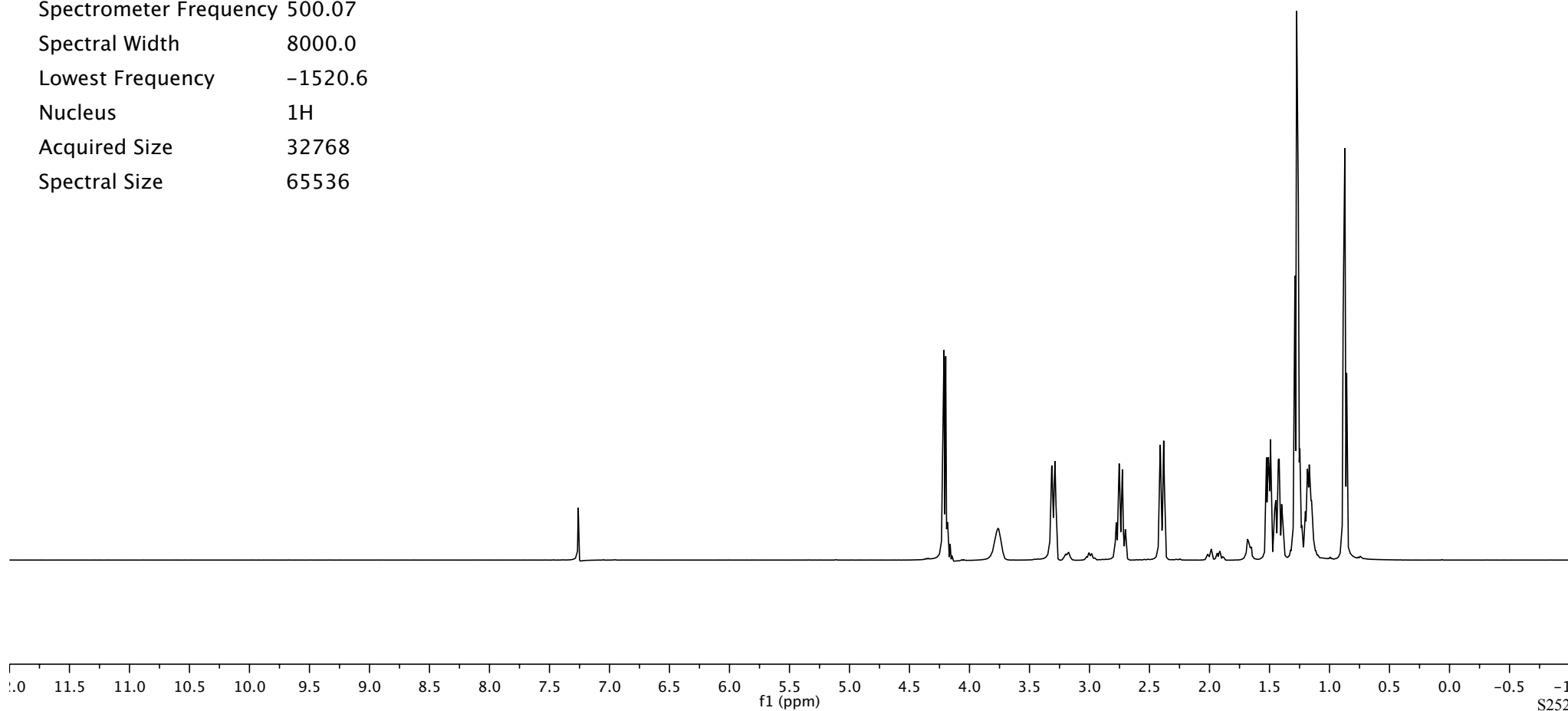
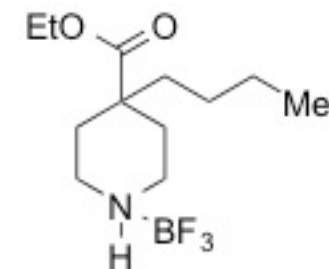


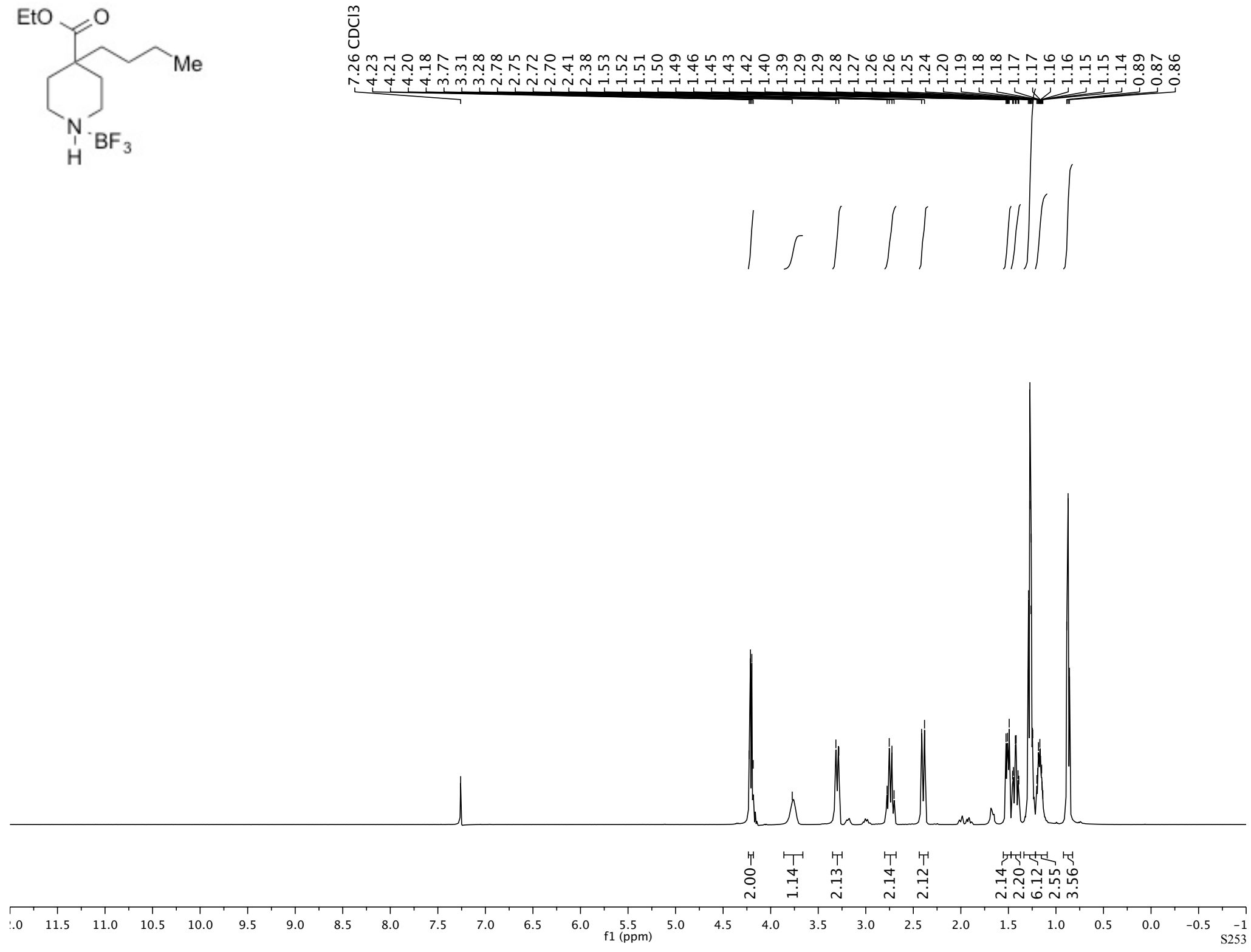
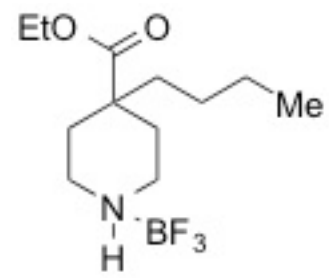


158.20
158.23
158.27

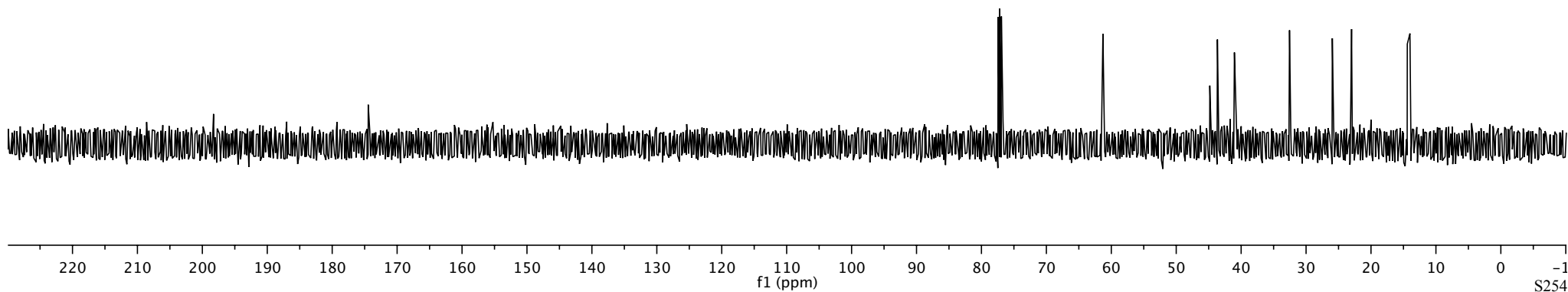
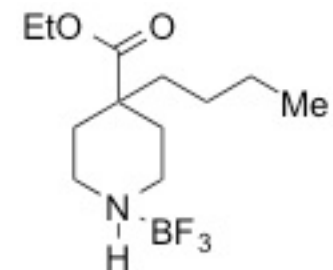


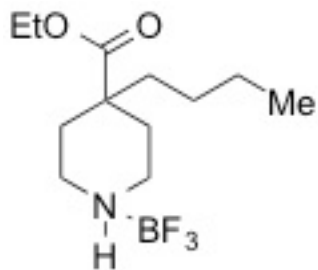
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	26
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1520.6
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536





Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	222
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1270.5
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536





—174.45

—77.16 CDCl₃

—61.29

—44.82

—43.65

—41.03

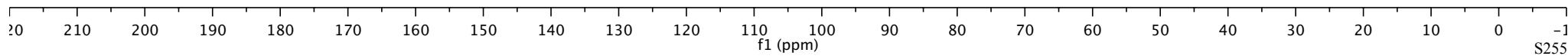
—32.54

—25.95

—22.99

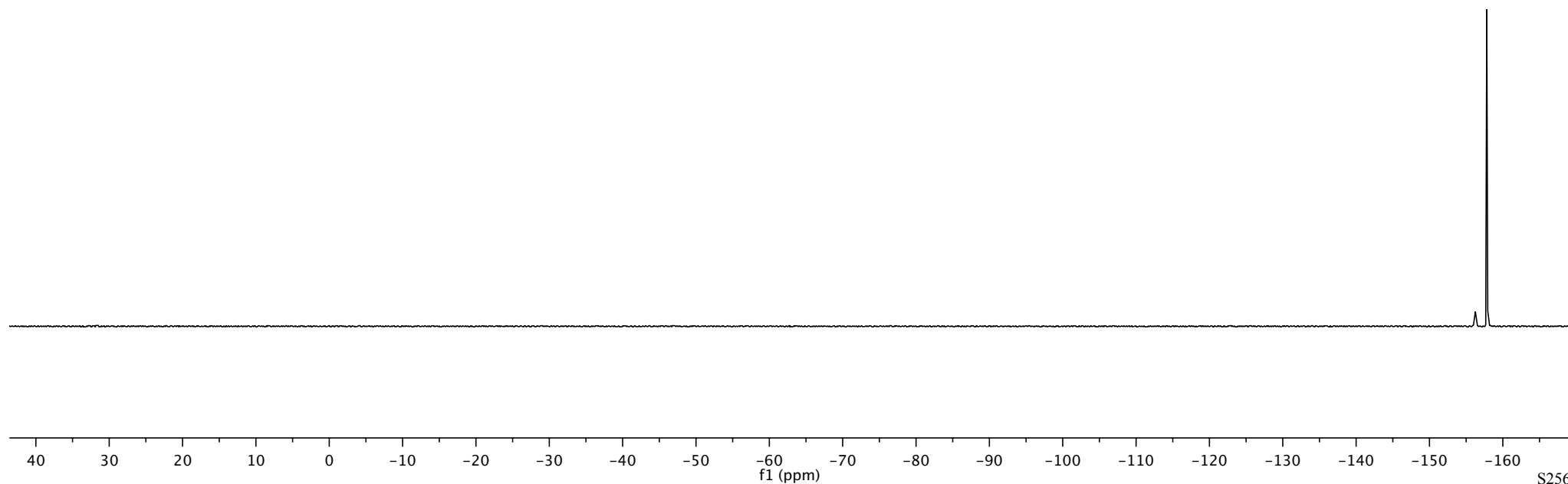
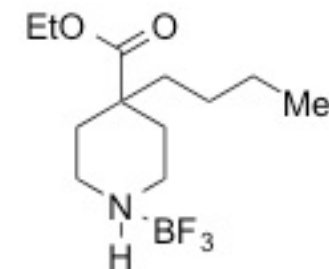
—14.40

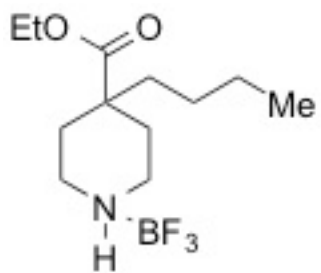
—14.00



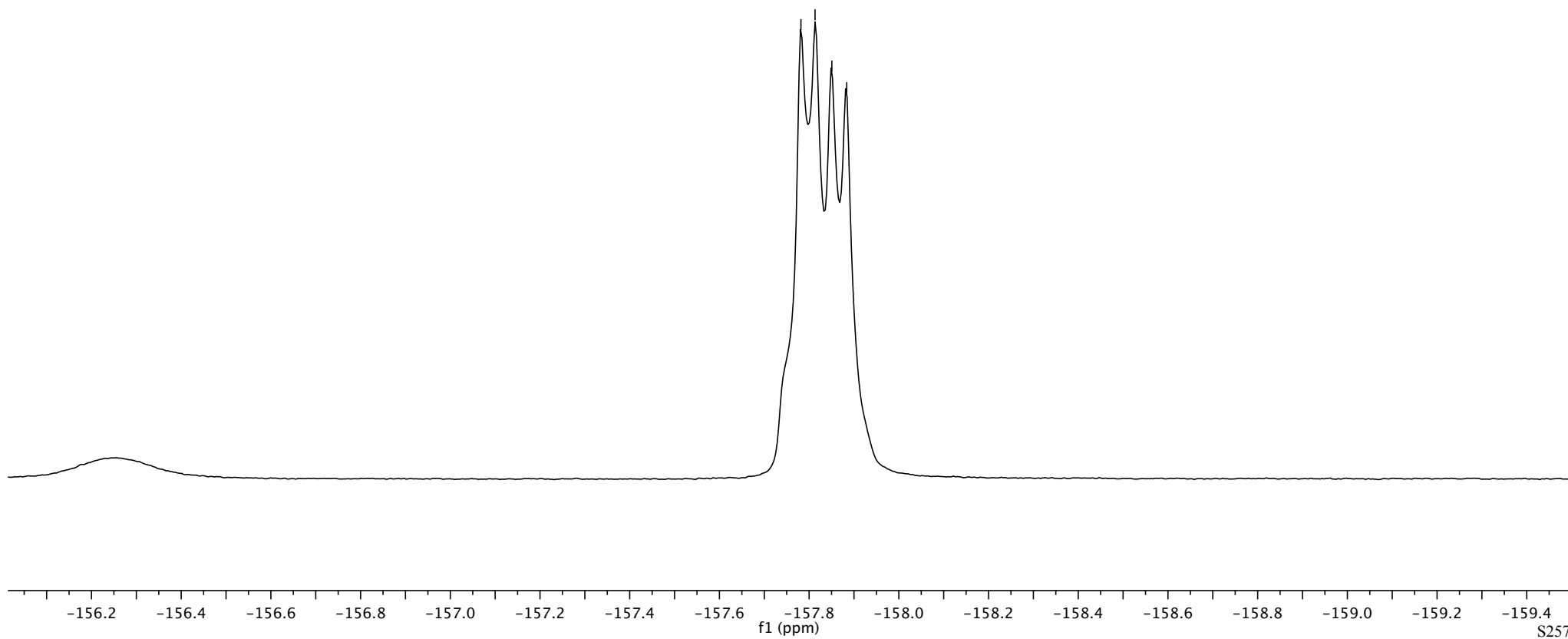
KF-IV-65_19F
7.30.2015
KF-IV-65_19F

Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	132
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency	-79501.3
Nucleus	19F
Acquired Size	32768
Spectral Size	65536

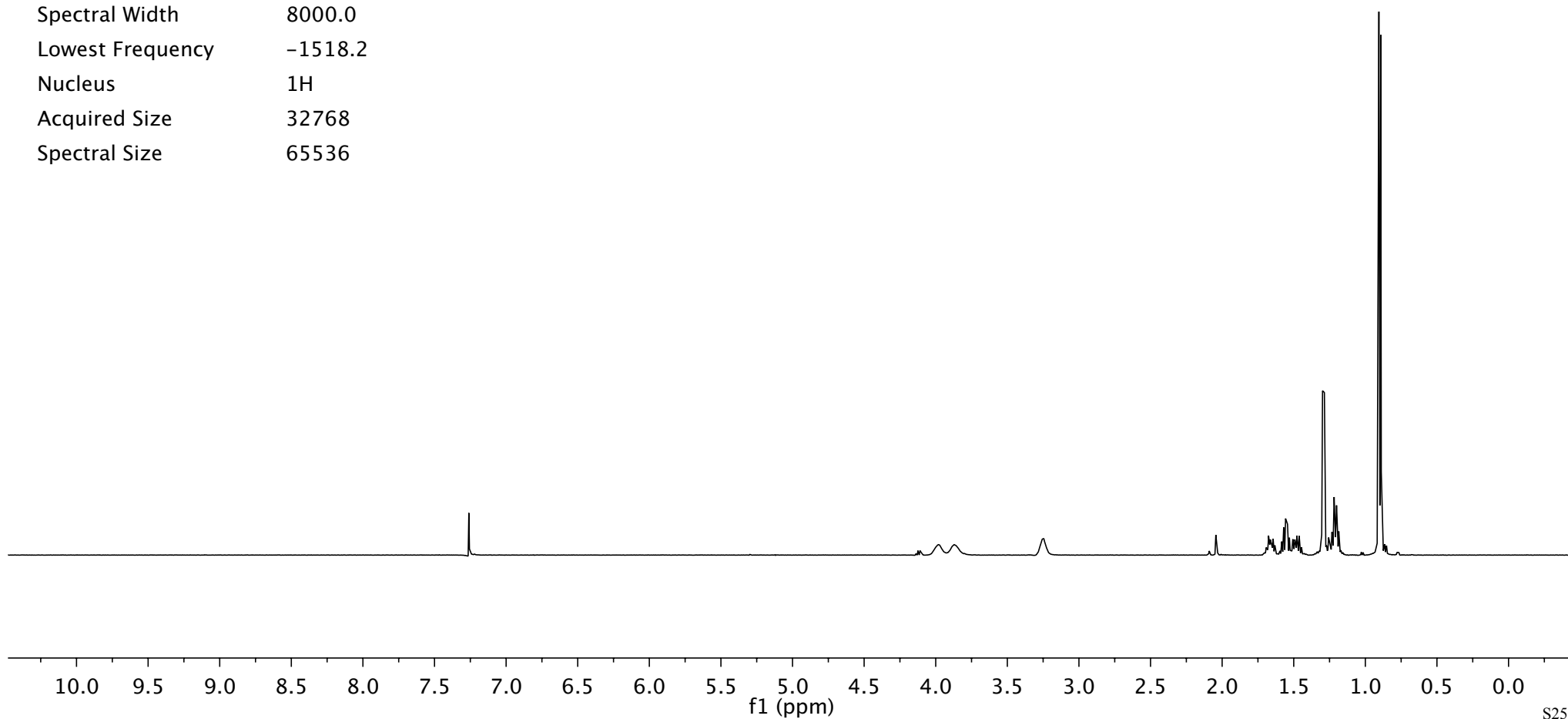
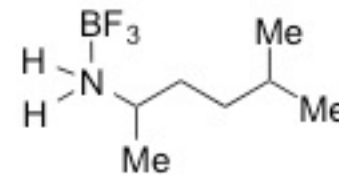


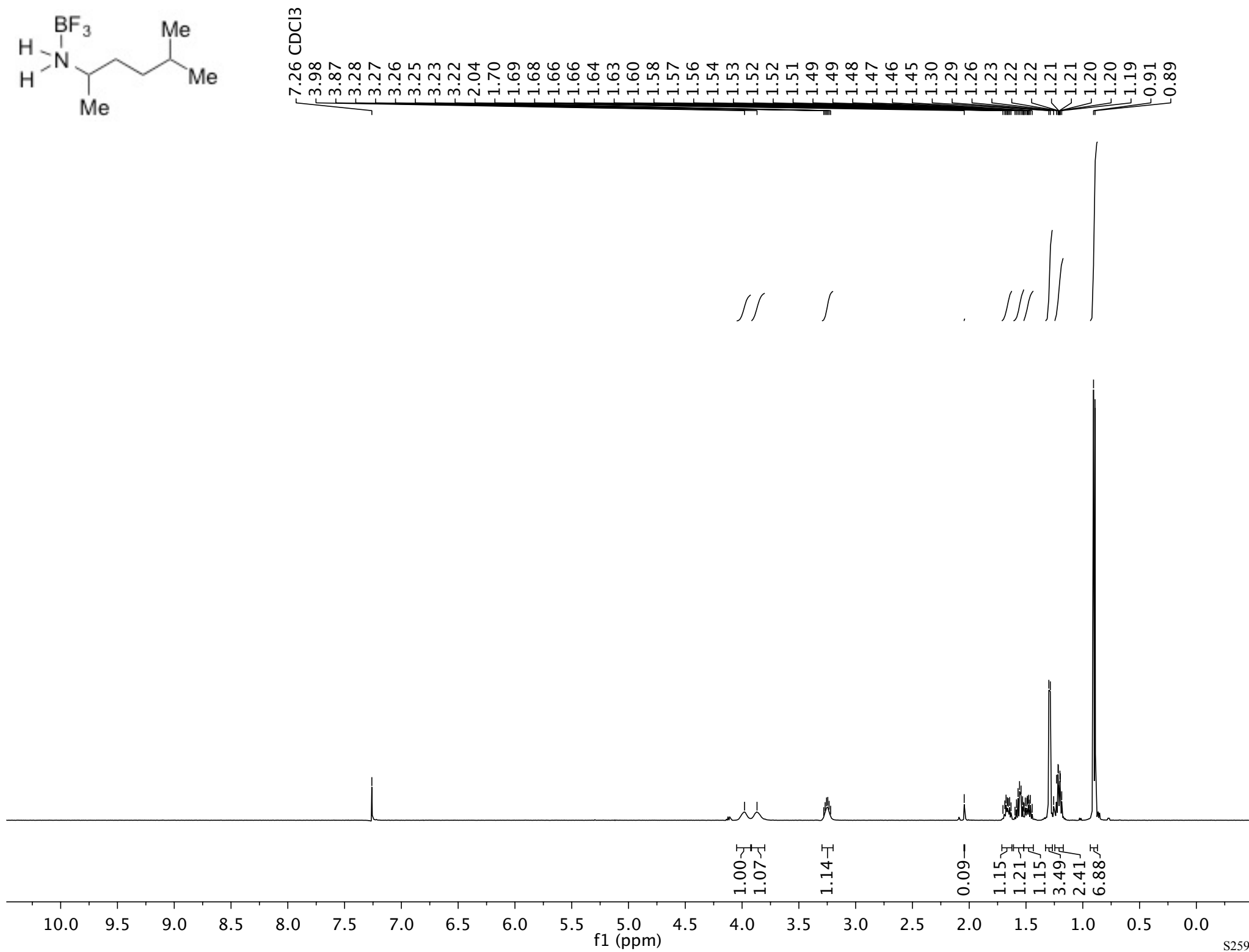
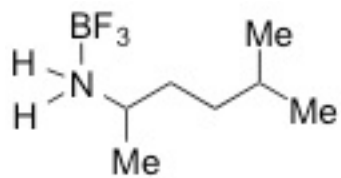


157.78
157.81
157.85
157.88

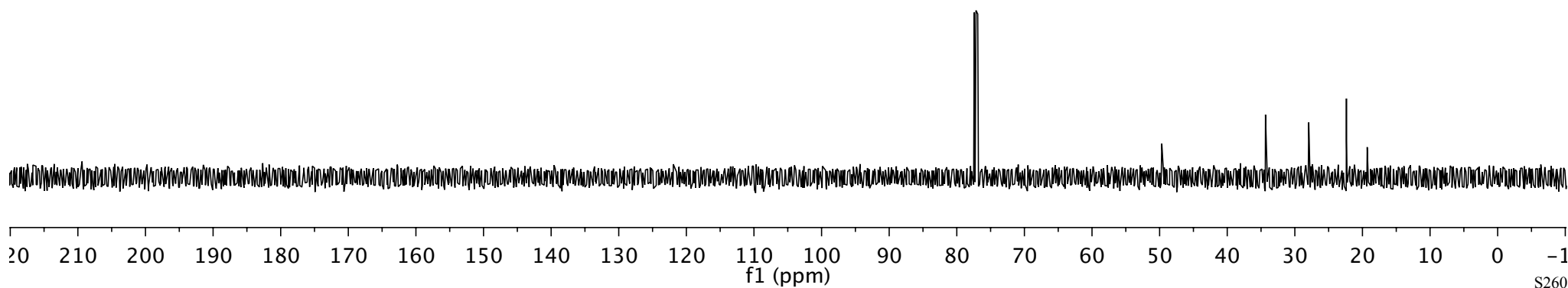
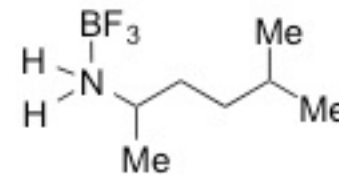


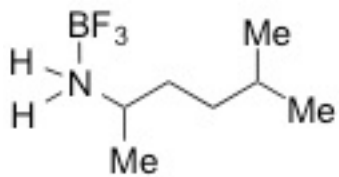
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	52
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	499.43
Spectral Width	8000.0
Lowest Frequency	-1518.2
Nucleus	1H
Acquired Size	32768
Spectral Size	65536





Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2200.7
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

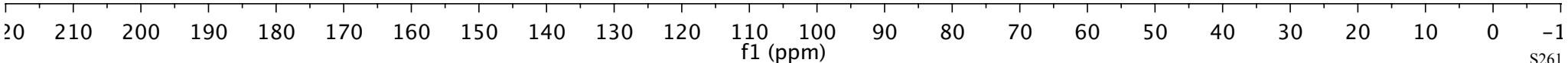




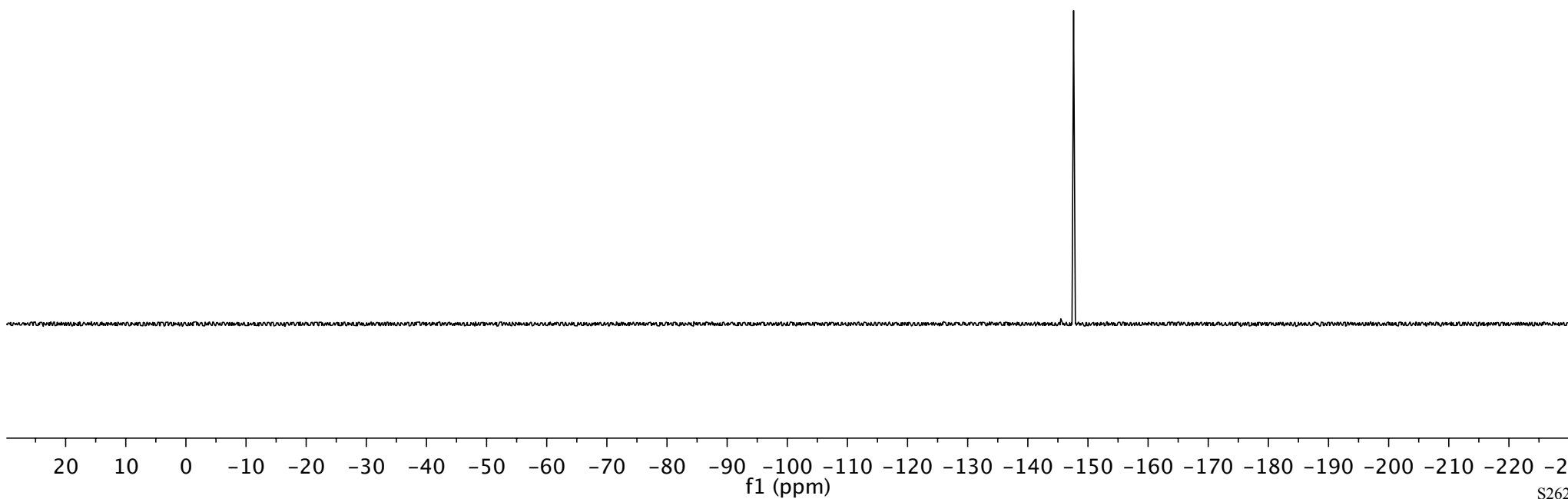
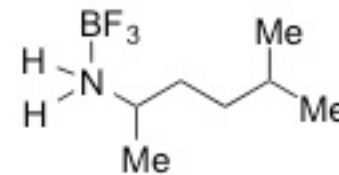
77.42 CDCl3
77.16 CDCl3
76.91 CDCl3

49.68

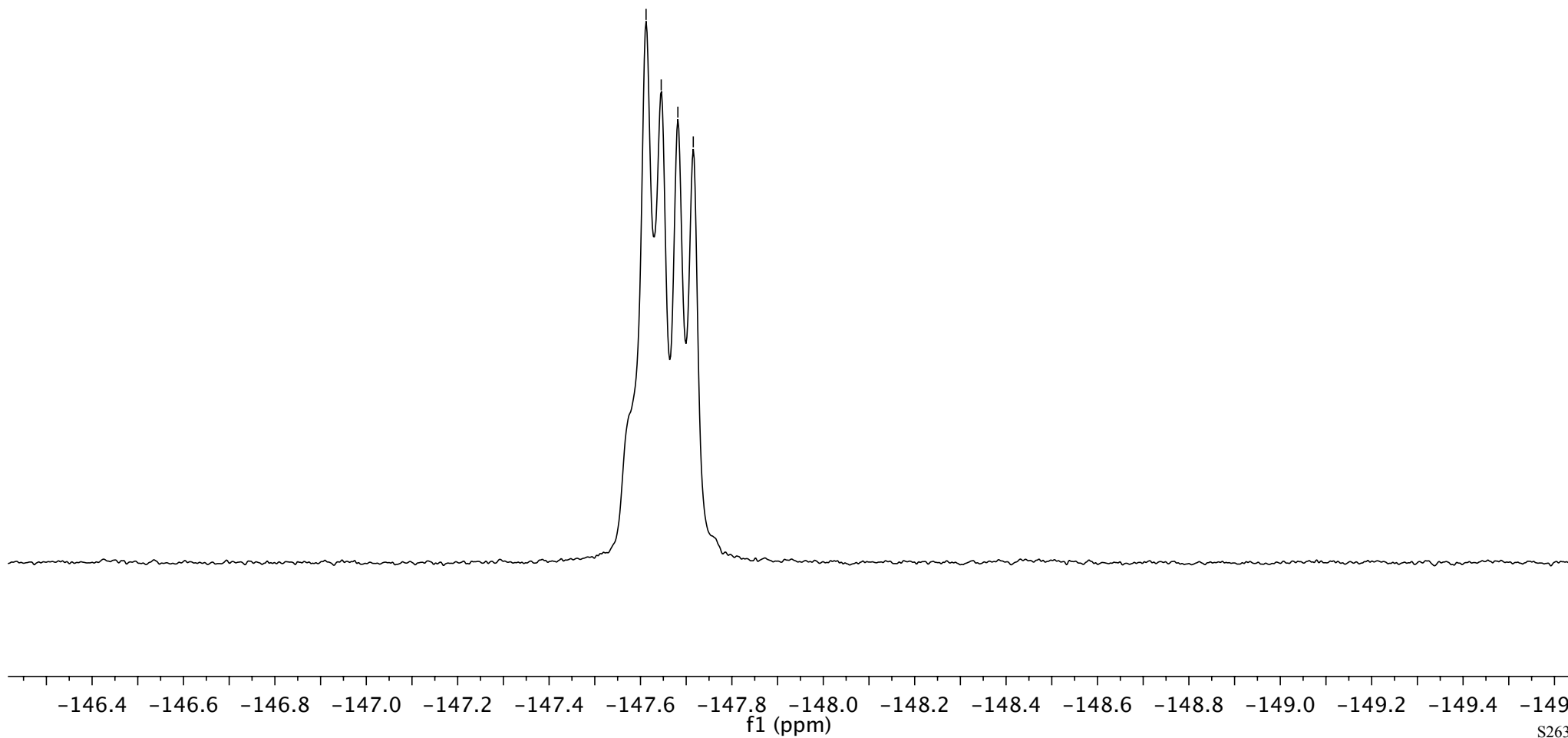
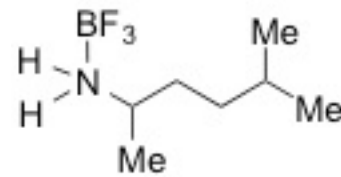
34.34
34.23
27.94
22.62
22.37
19.30



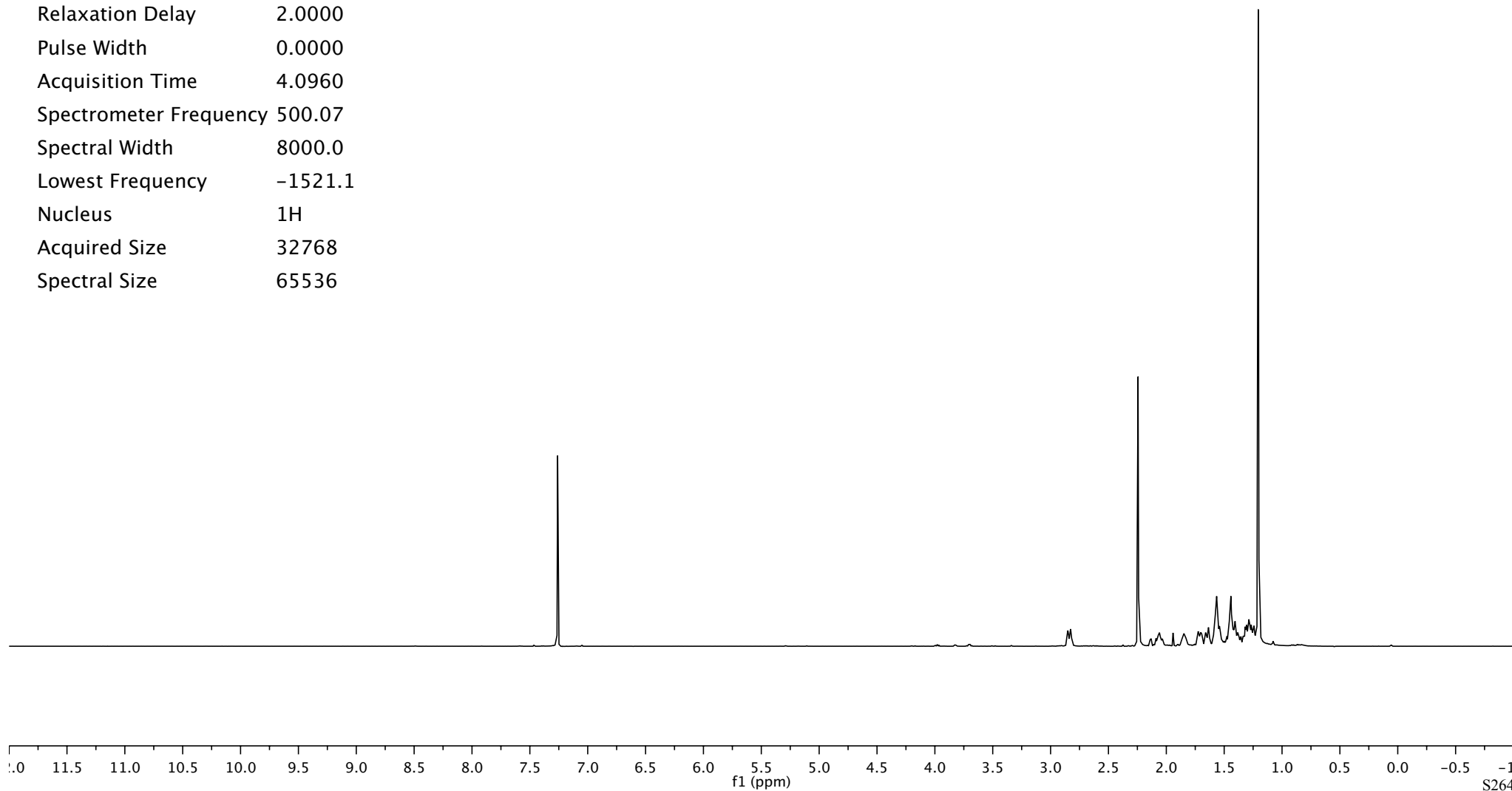
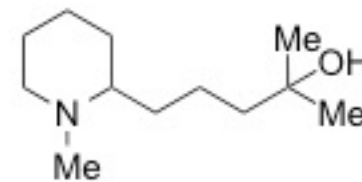
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	56
Relaxation Delay	1.5000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	469.89
Spectral Width	122137.4
Lowest Frequency	-108111.4
Nucleus	19F
Acquired Size	40022
Spectral Size	131072

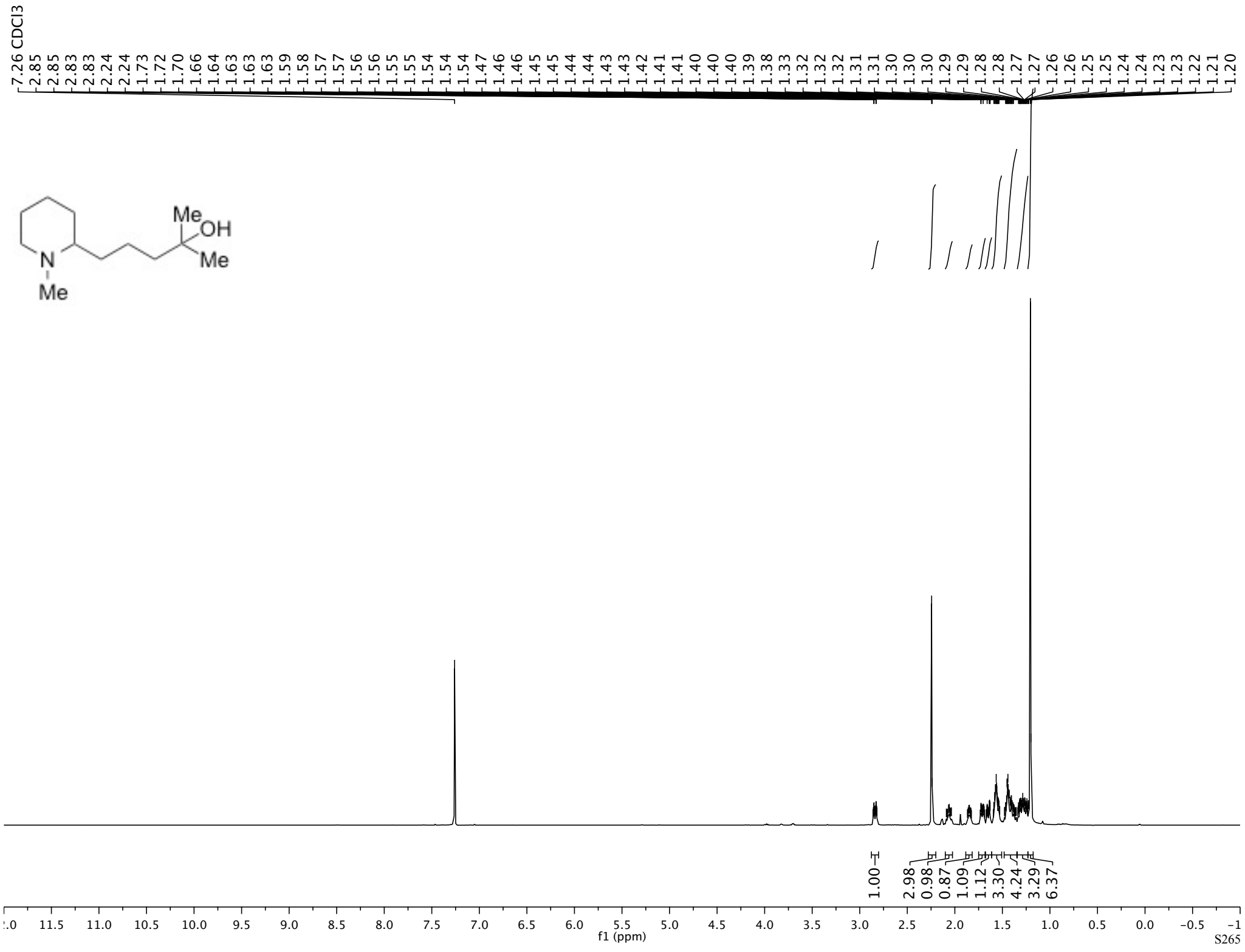


147.61
147.65
147.68
147.72

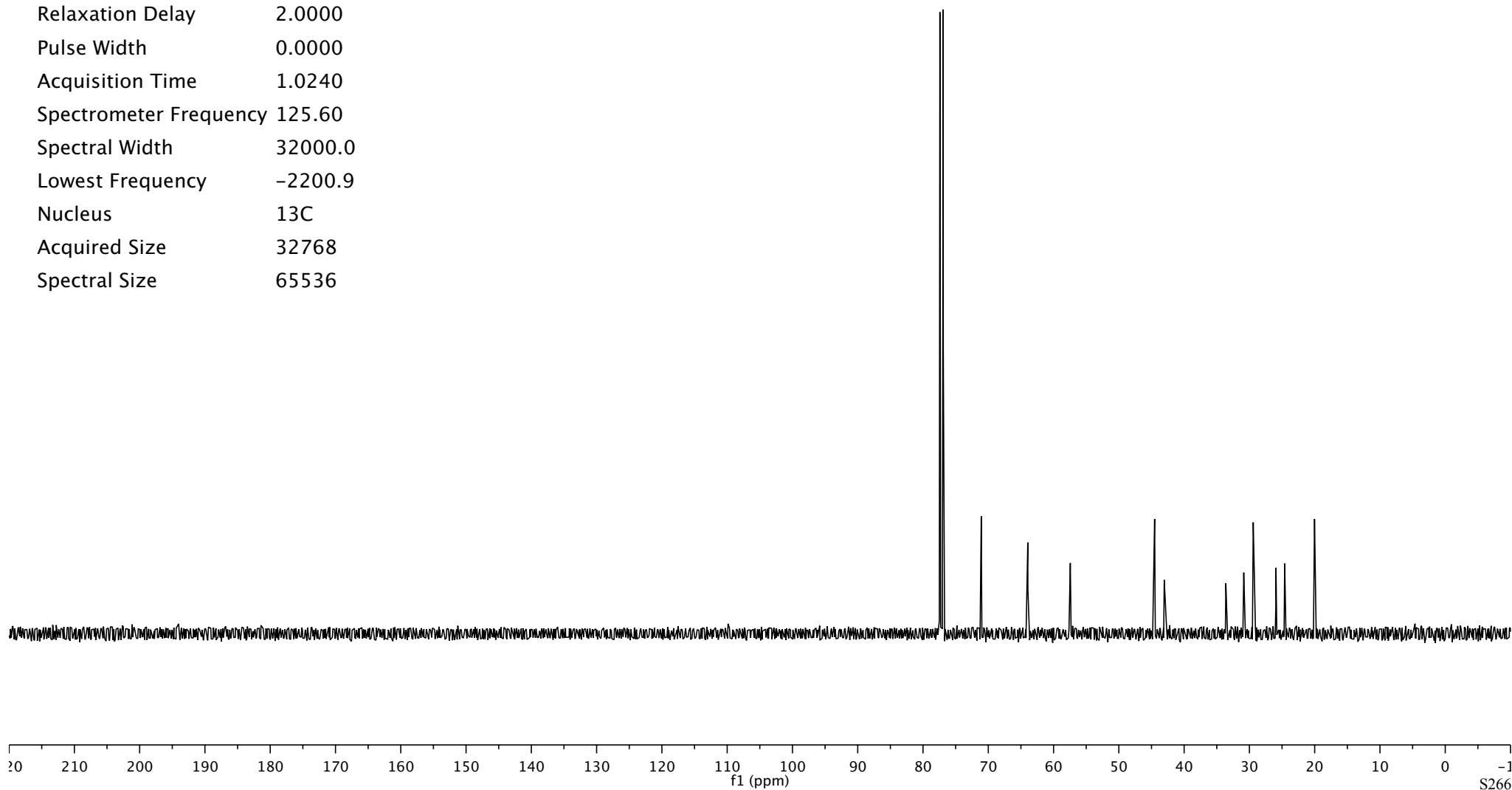
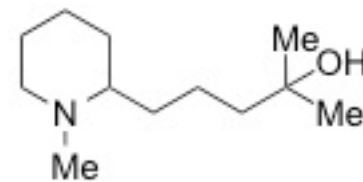


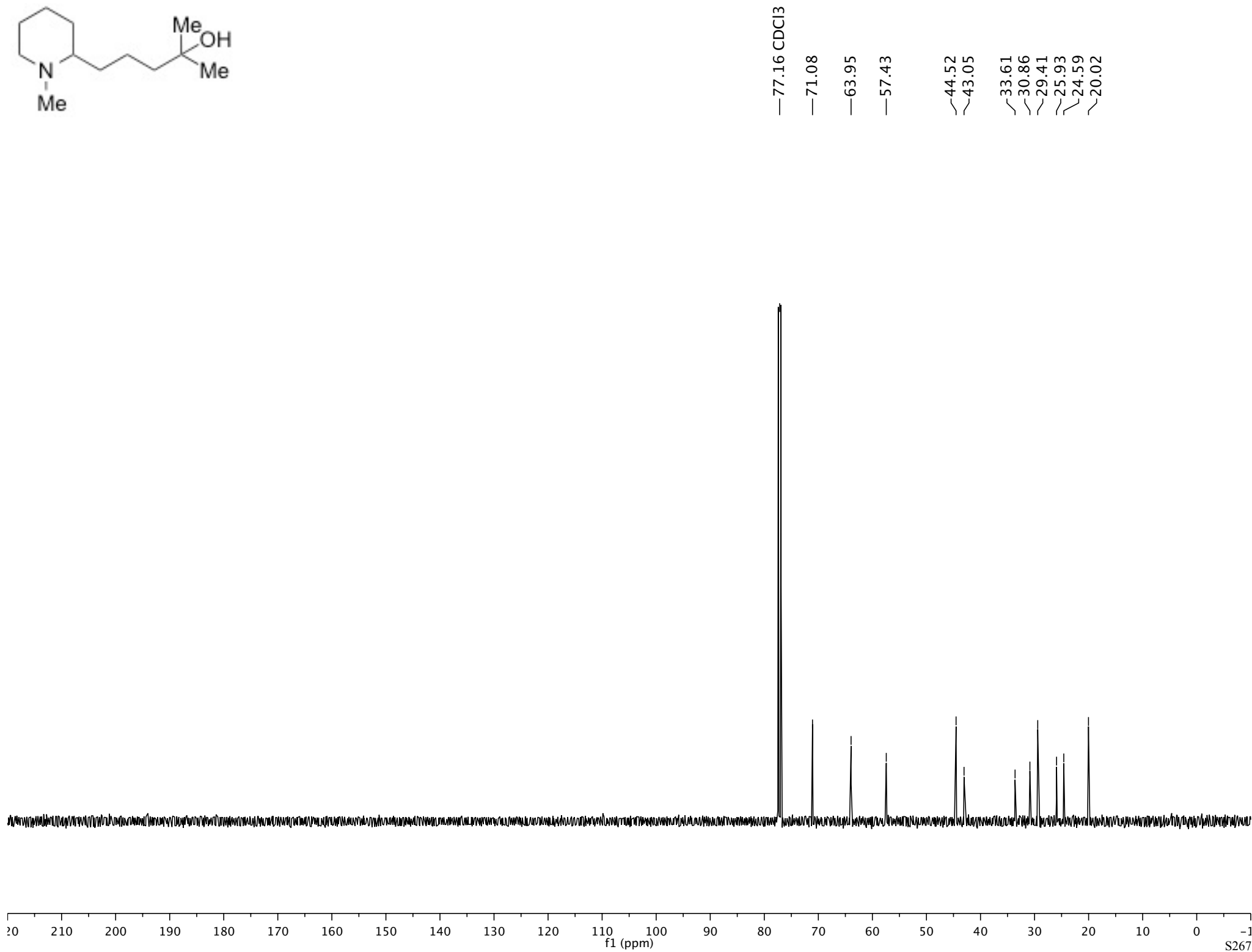
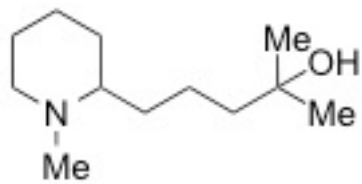
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	28
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



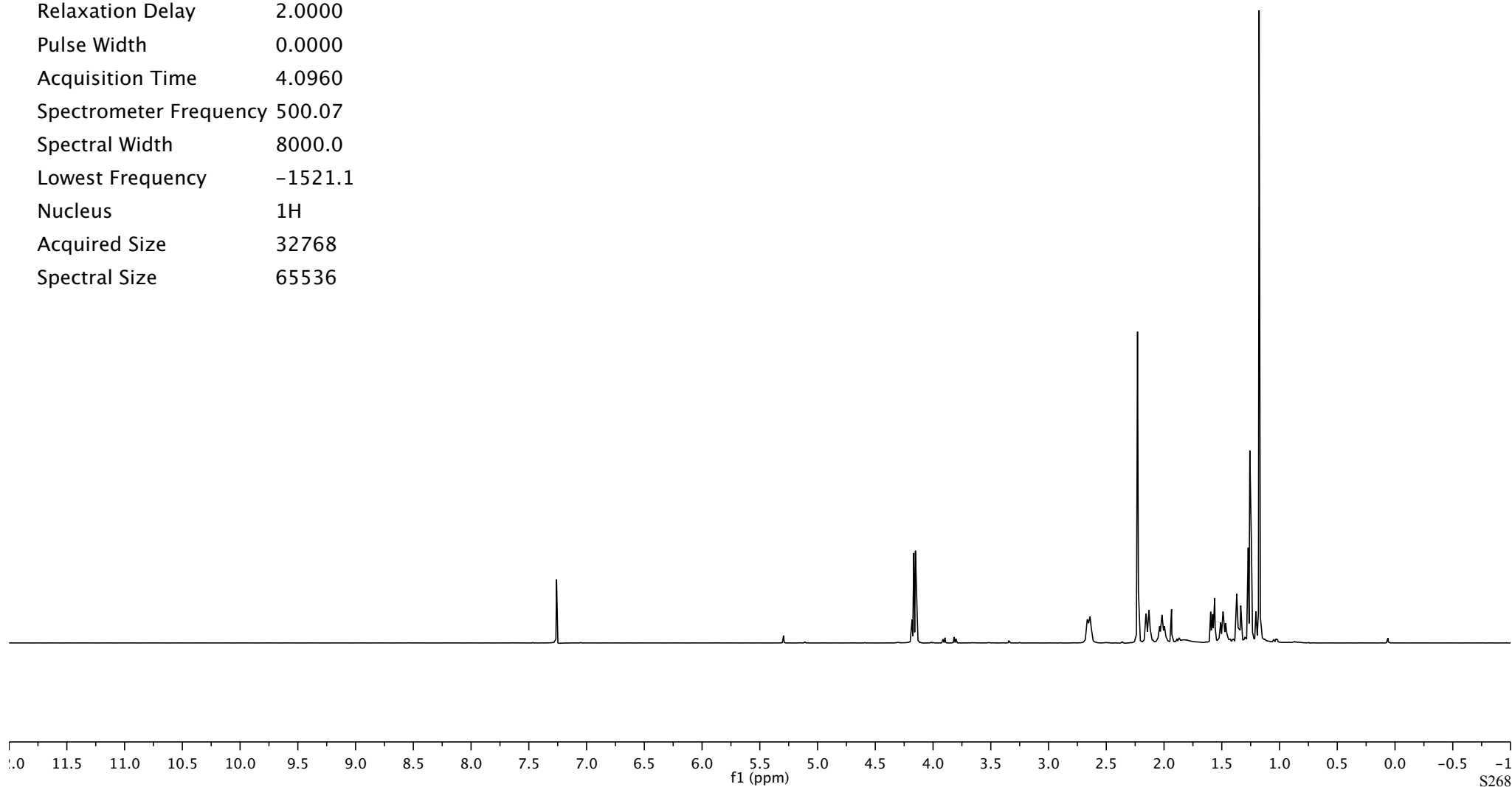
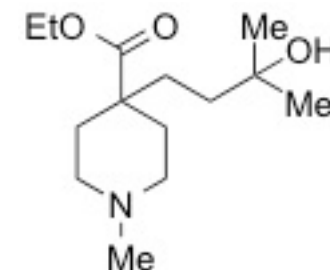


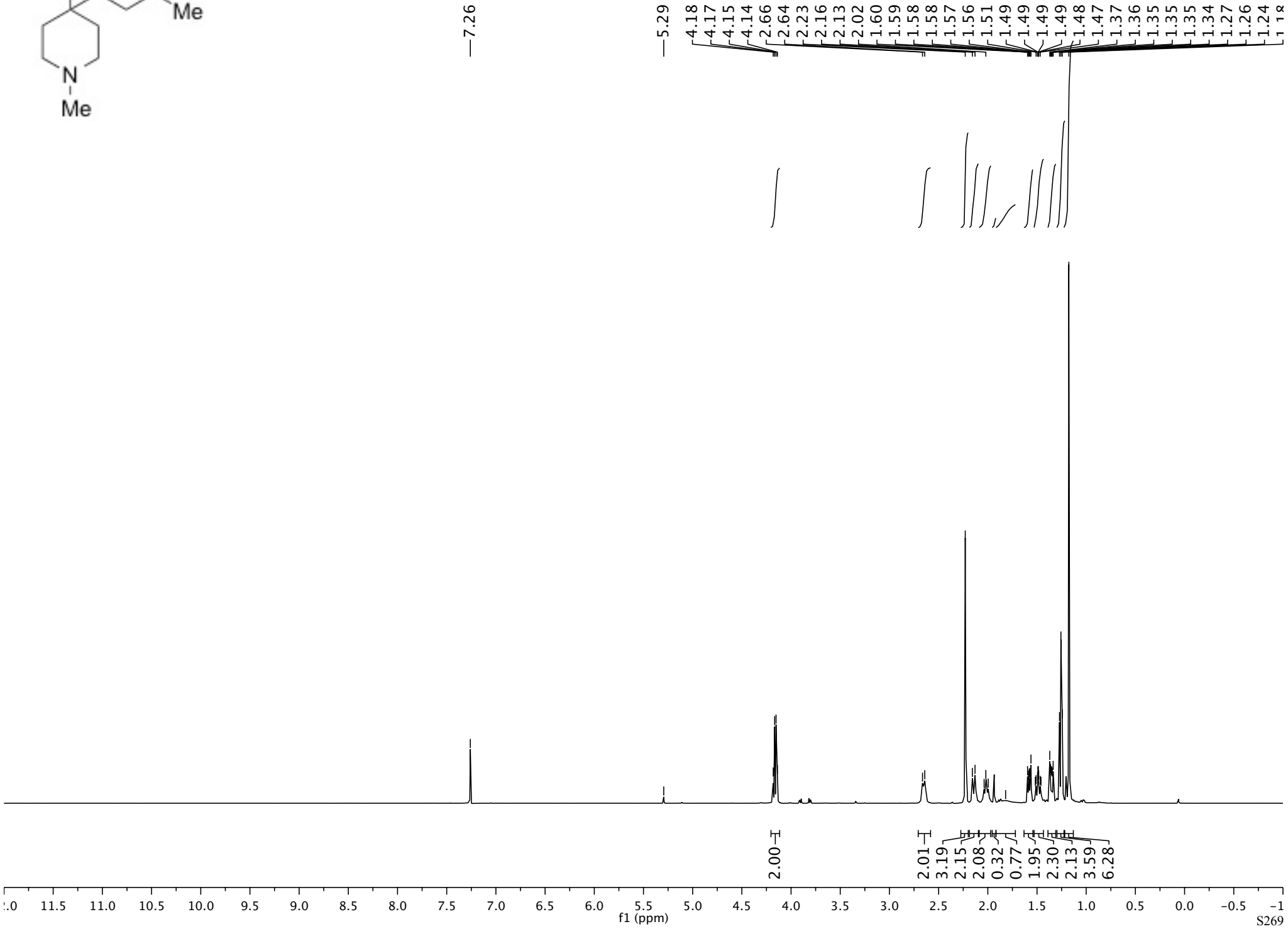
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Number of Scans	653
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2200.9
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536





Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	34
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

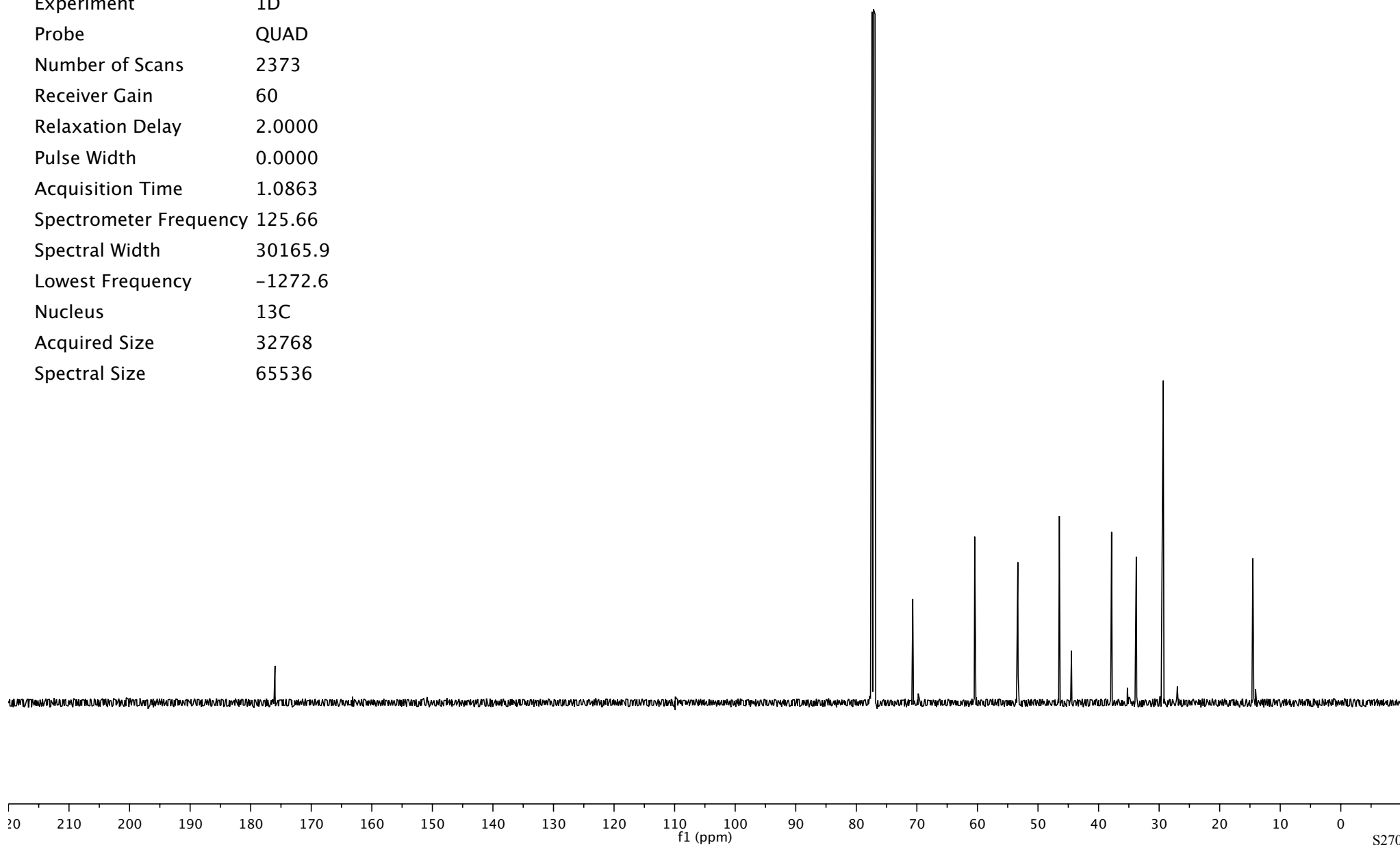
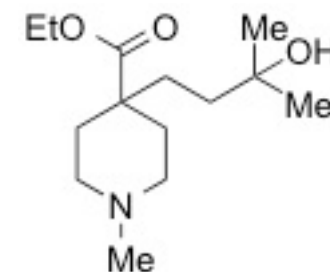


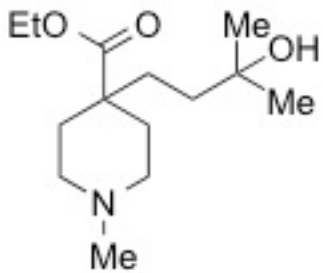


—5.29

2.01
3.19
2.15
2.08
0.32
0.77
1.95
2.30
2.13
3.59
6.28

Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	2373
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1272.6
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536





—175.99

—77.16 CDCl₃

—70.68

—60.44

—53.33

—46.47

—44.48

—37.85

—35.24

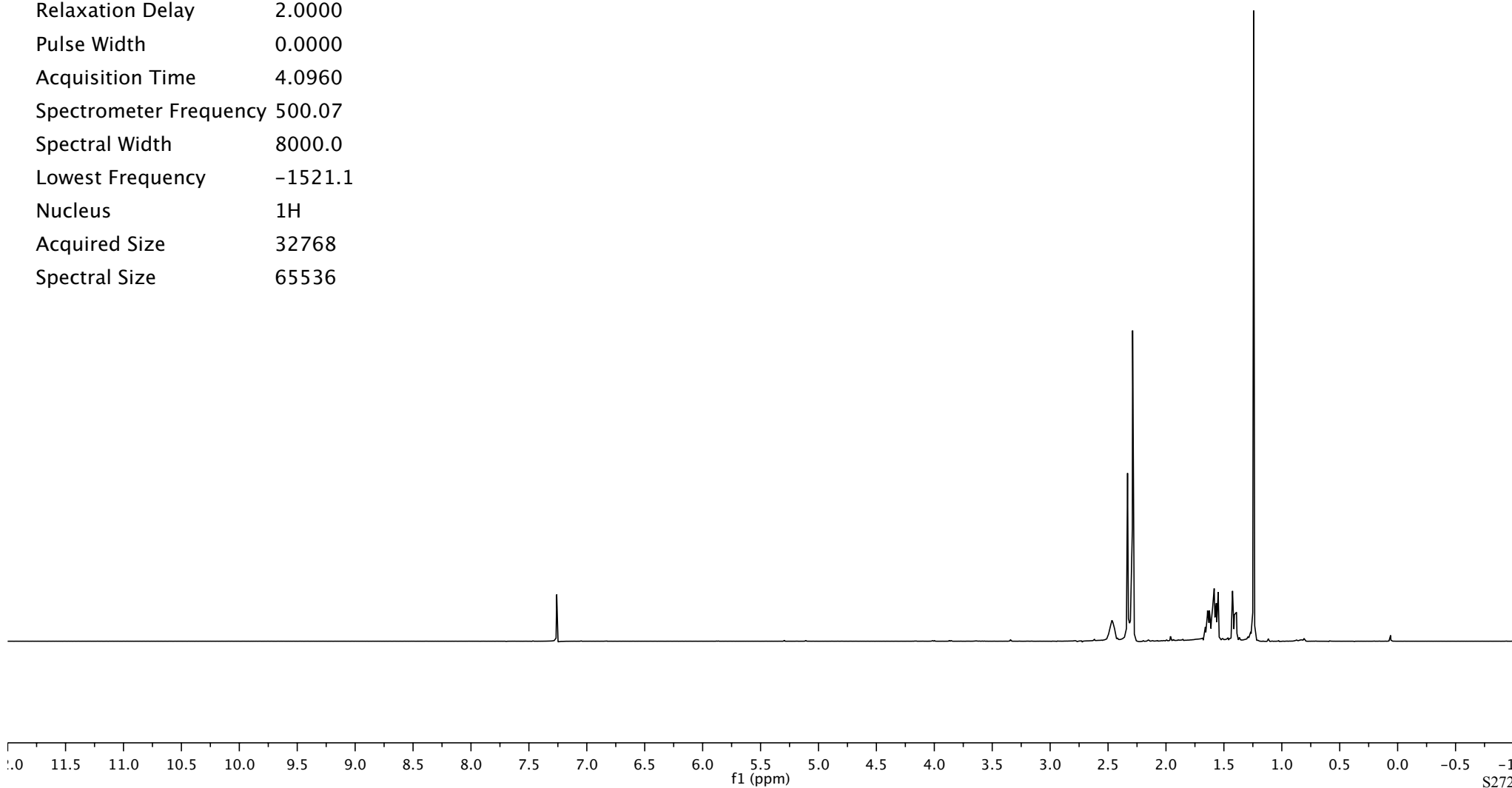
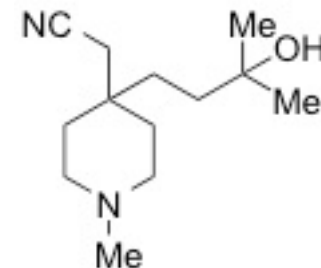
—33.78

—29.32

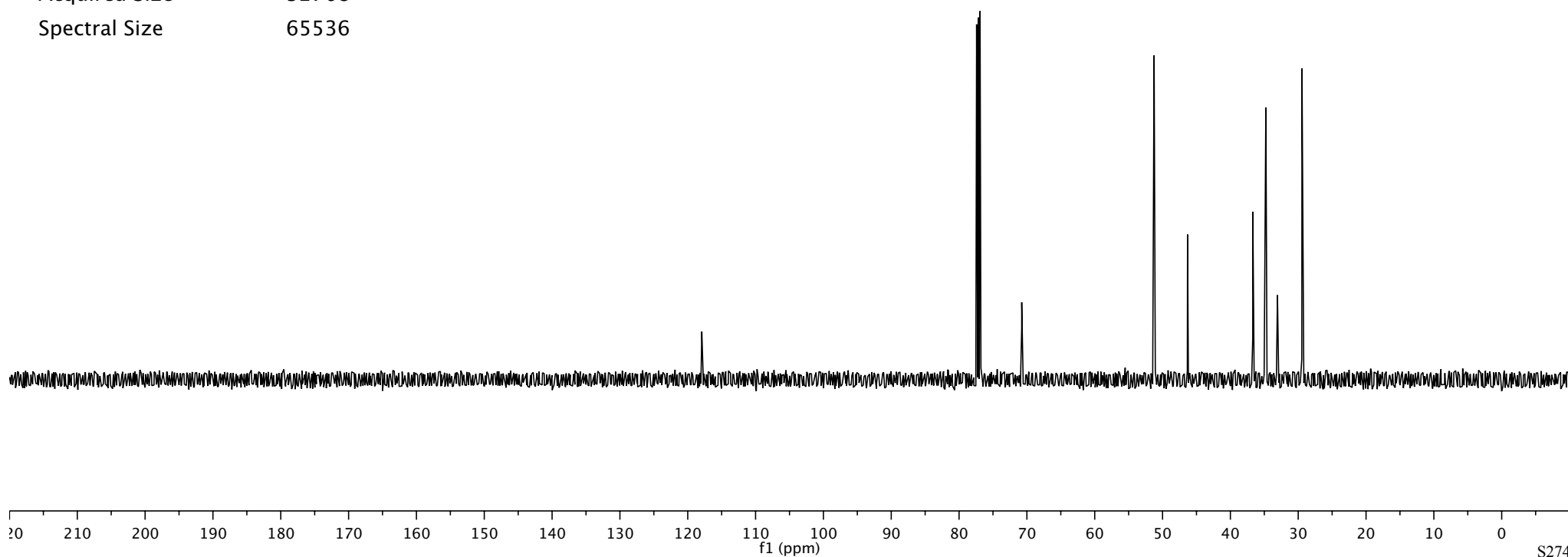
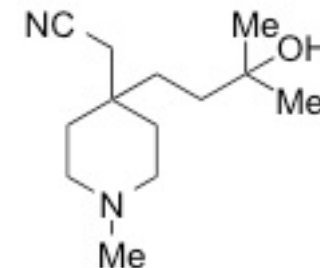
—14.53

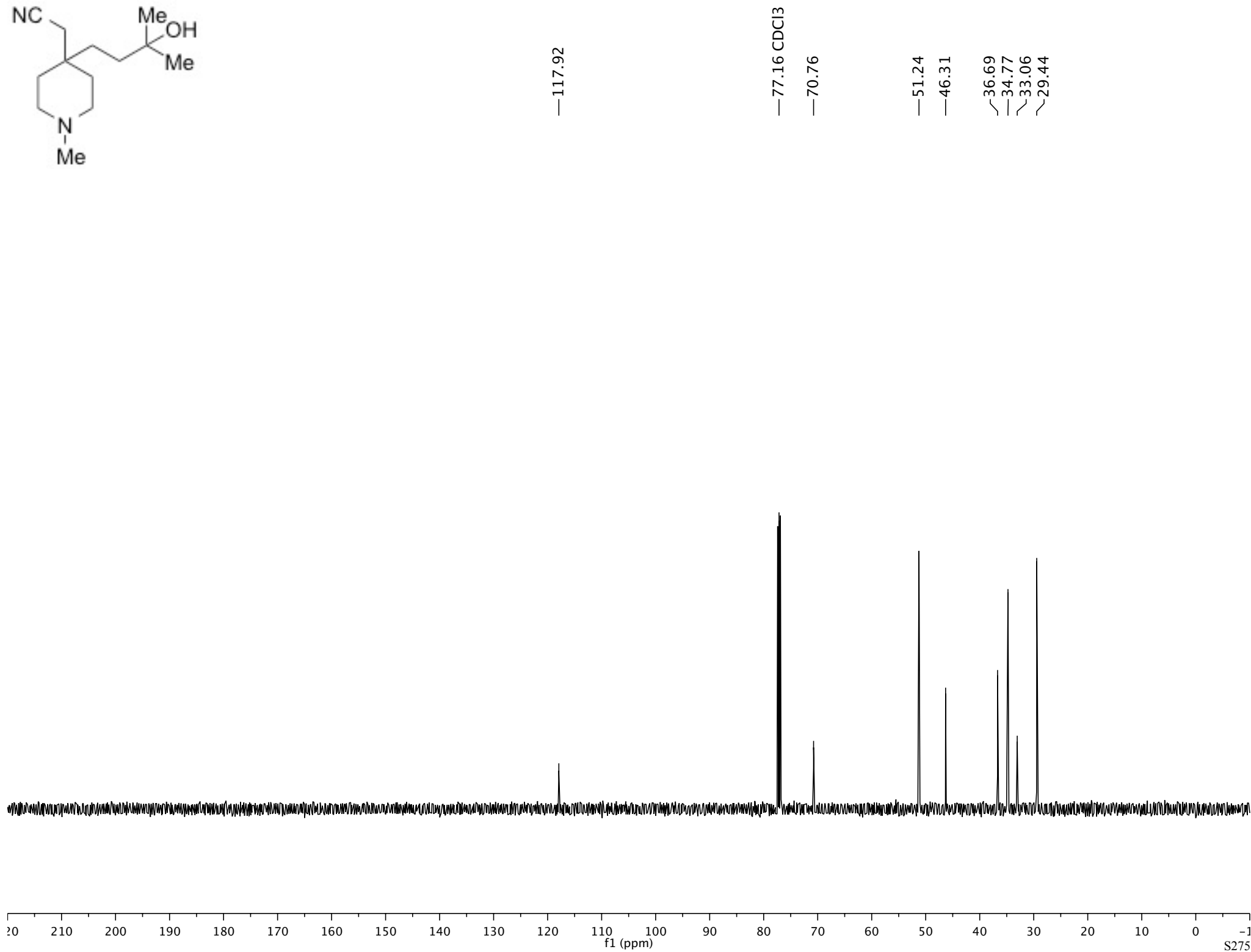
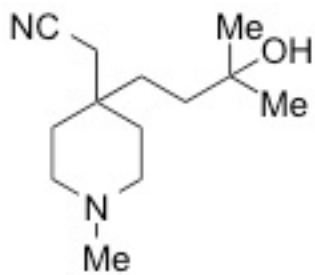
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm) S271

Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	32
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

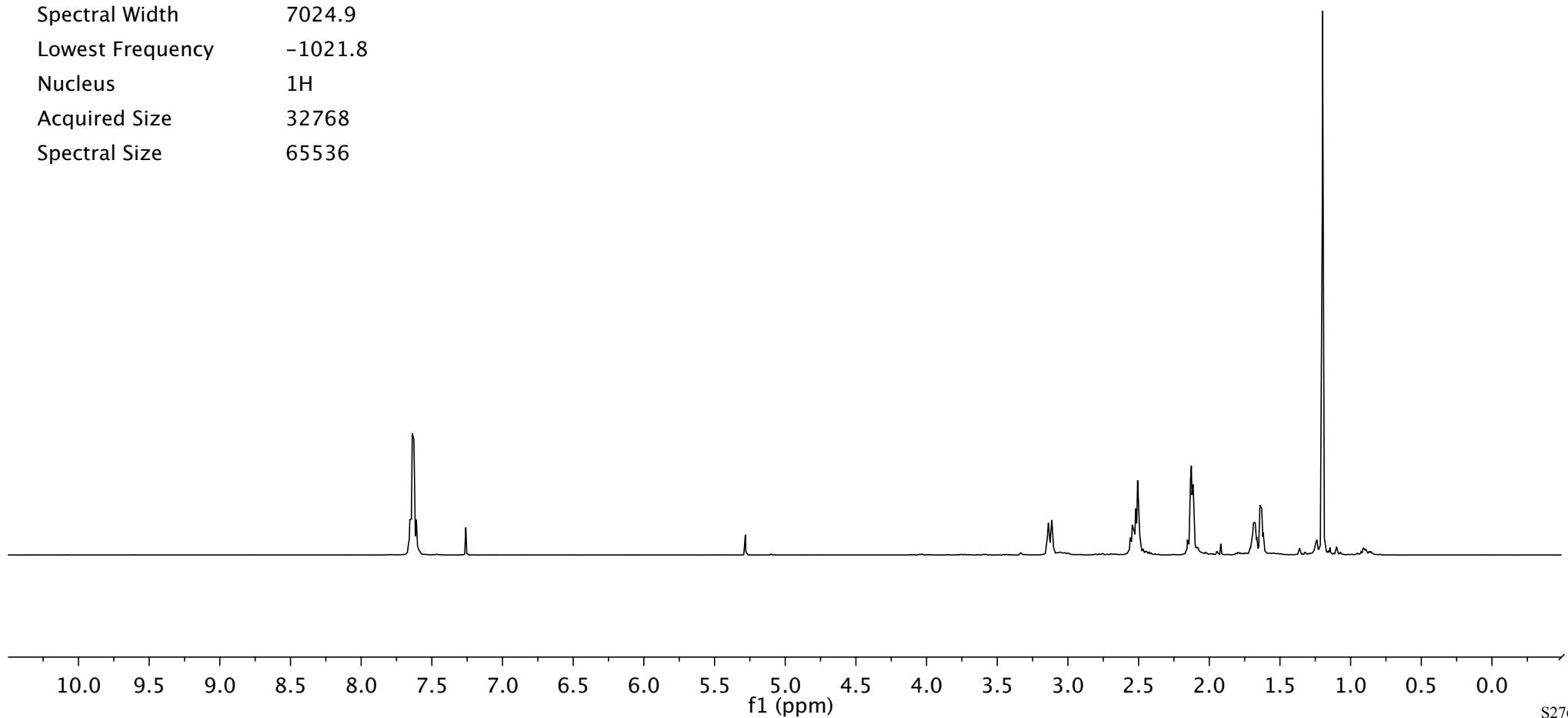
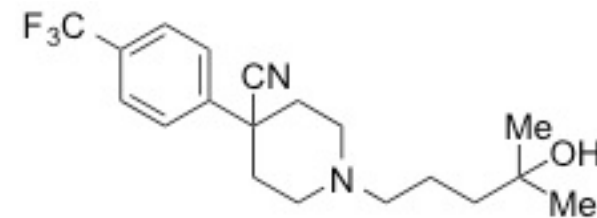


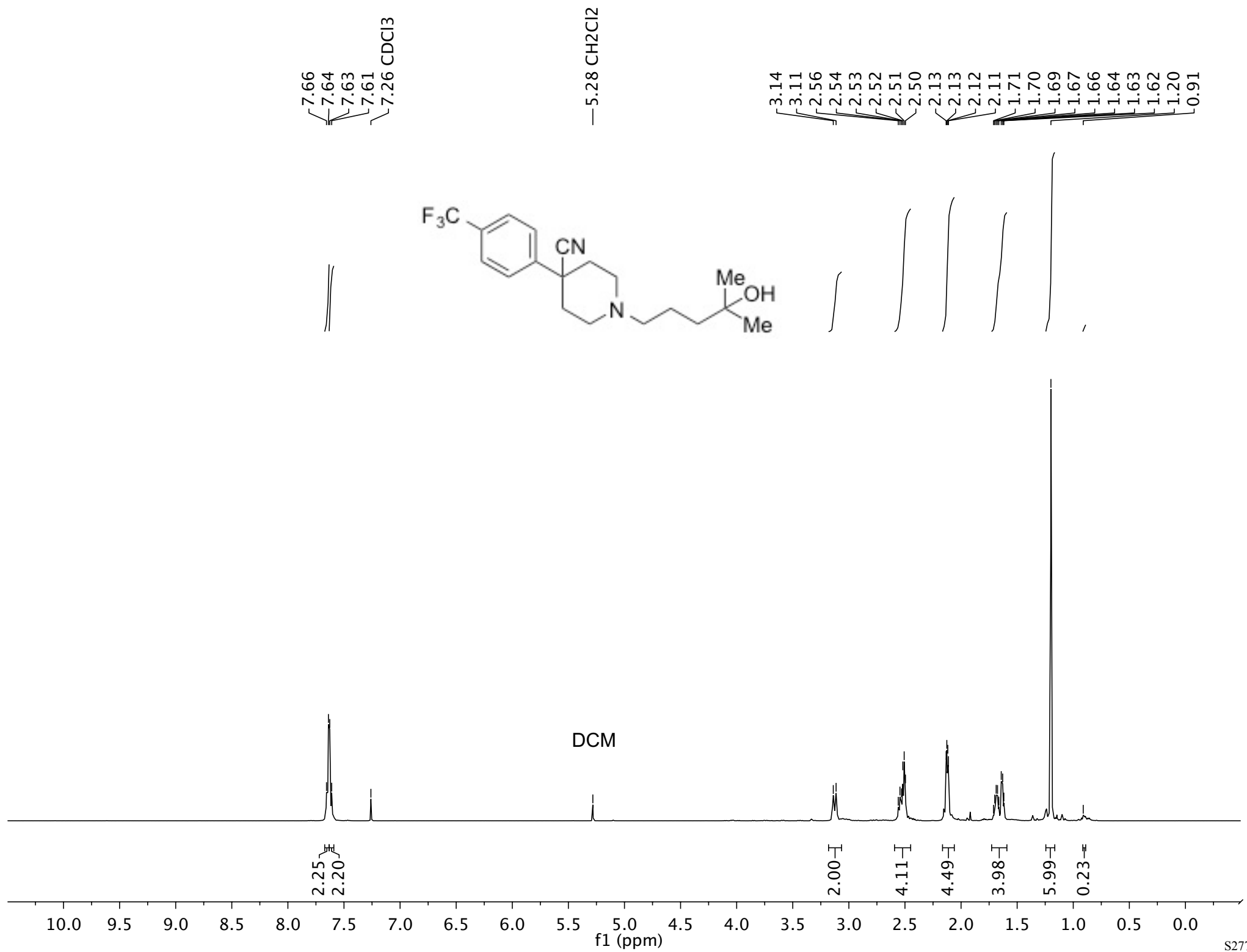
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	662
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1273.1
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



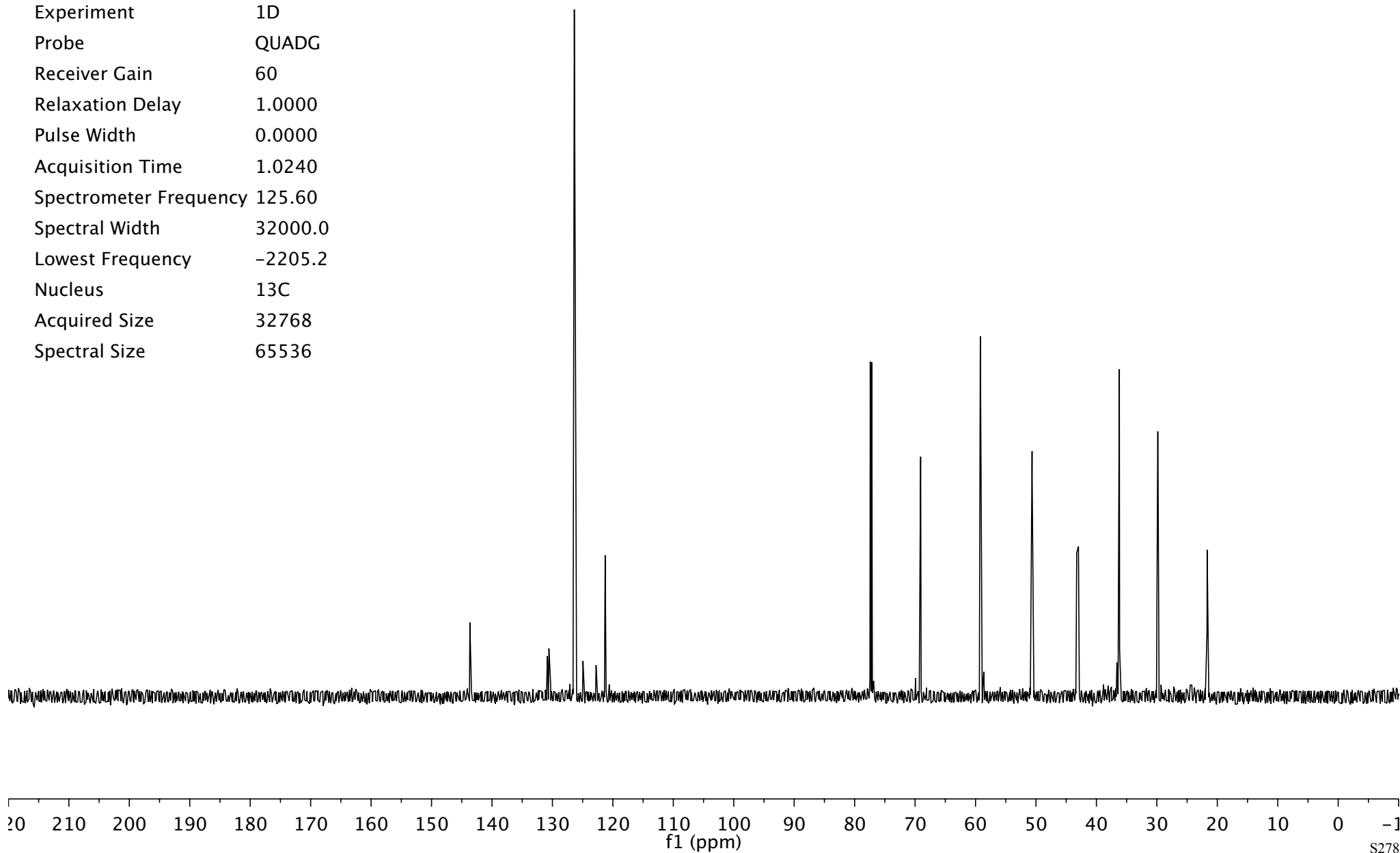
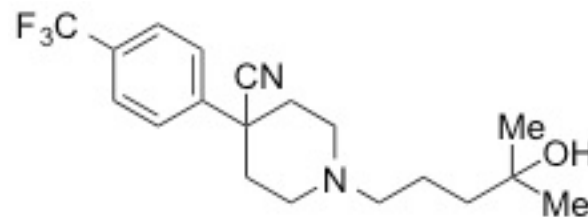


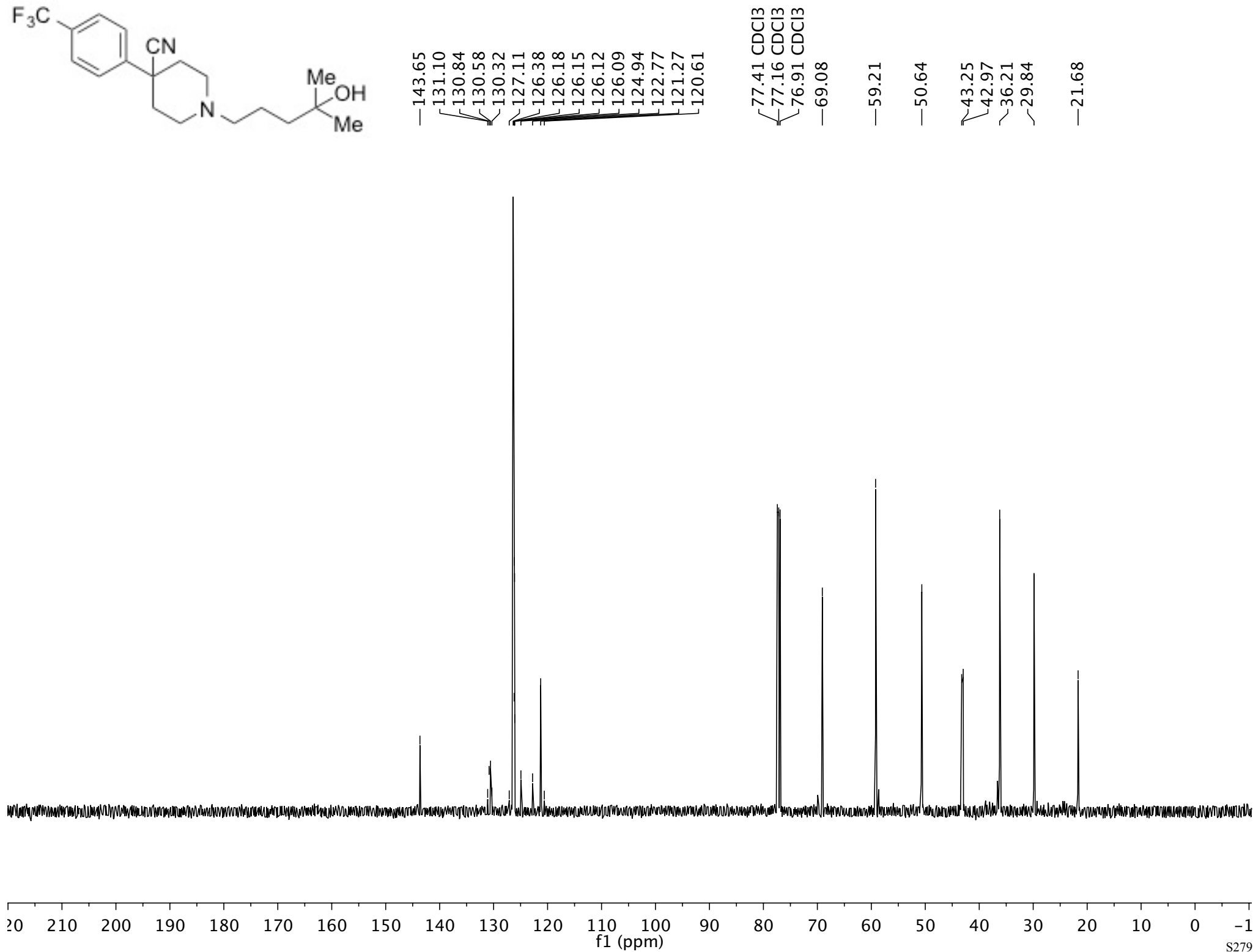
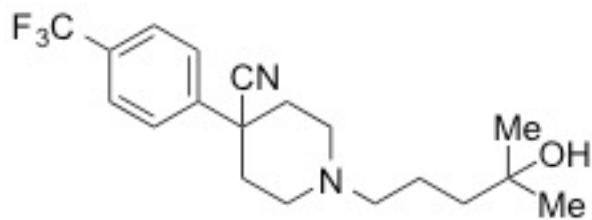
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	41
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.69
Spectral Width	7024.9
Lowest Frequency	-1021.8
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



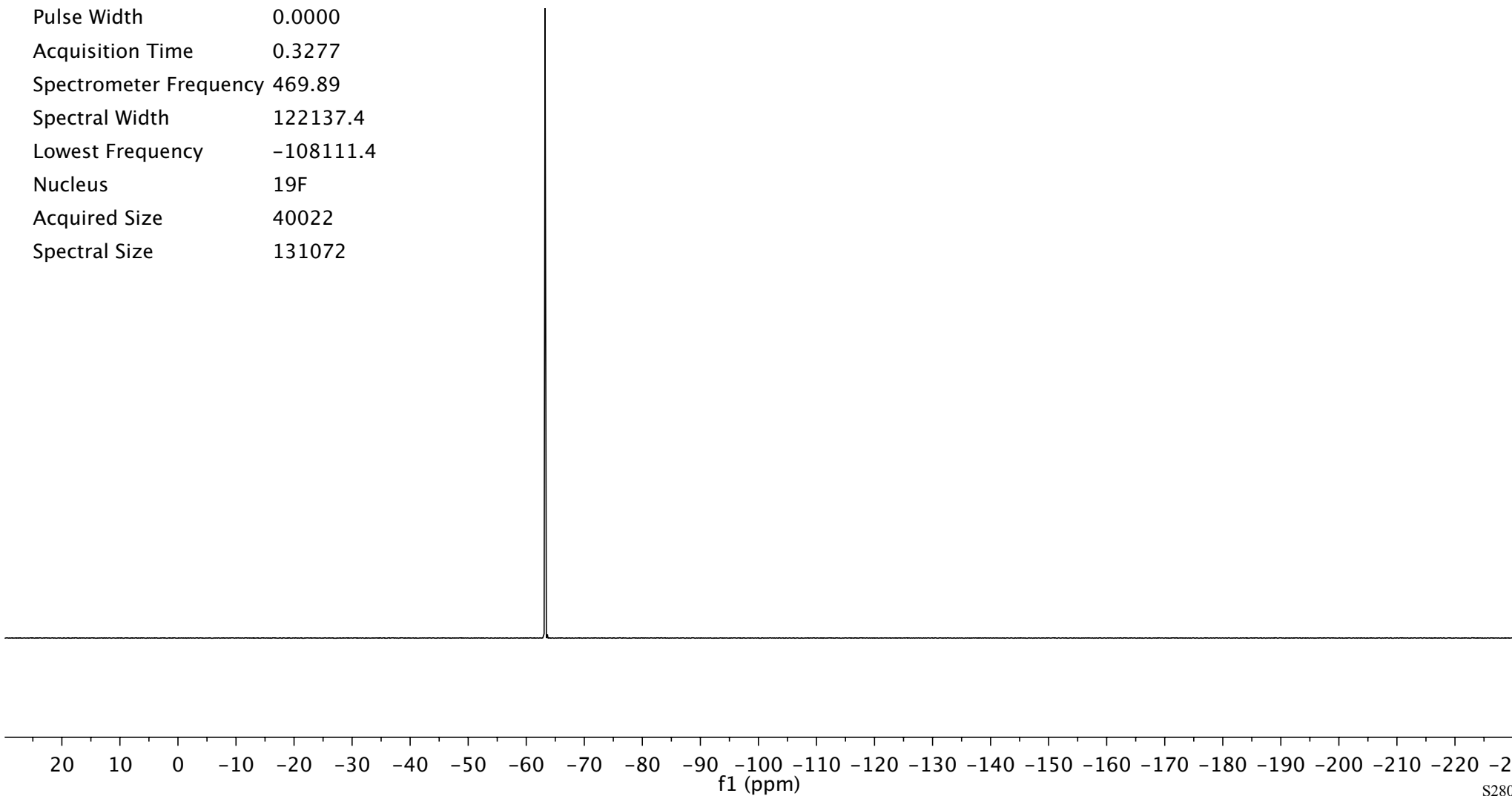
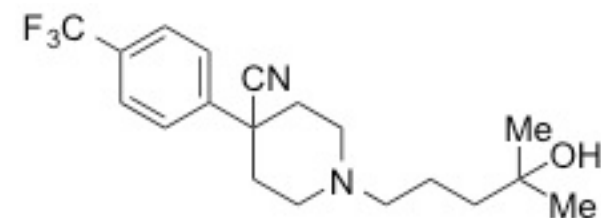


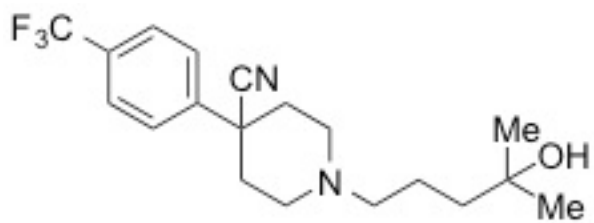
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2205.2
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536





Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	56
Relaxation Delay	1.5000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	469.89
Spectral Width	122137.4
Lowest Frequency	-108111.4
Nucleus	19F
Acquired Size	40022
Spectral Size	131072



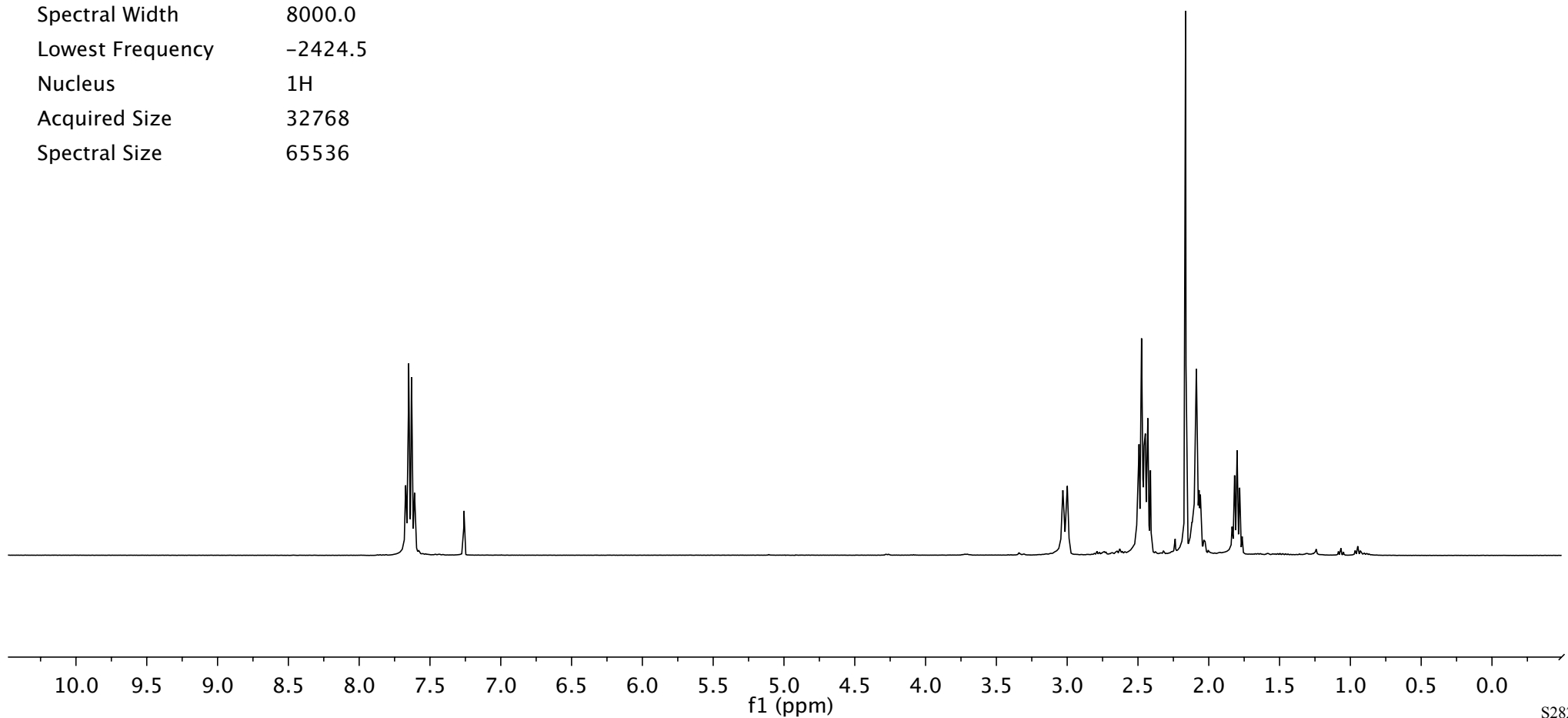
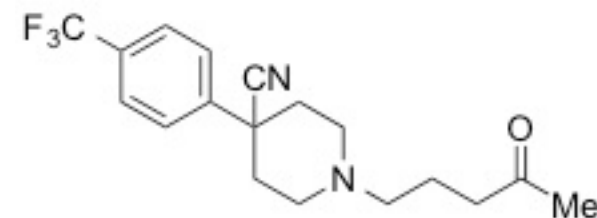


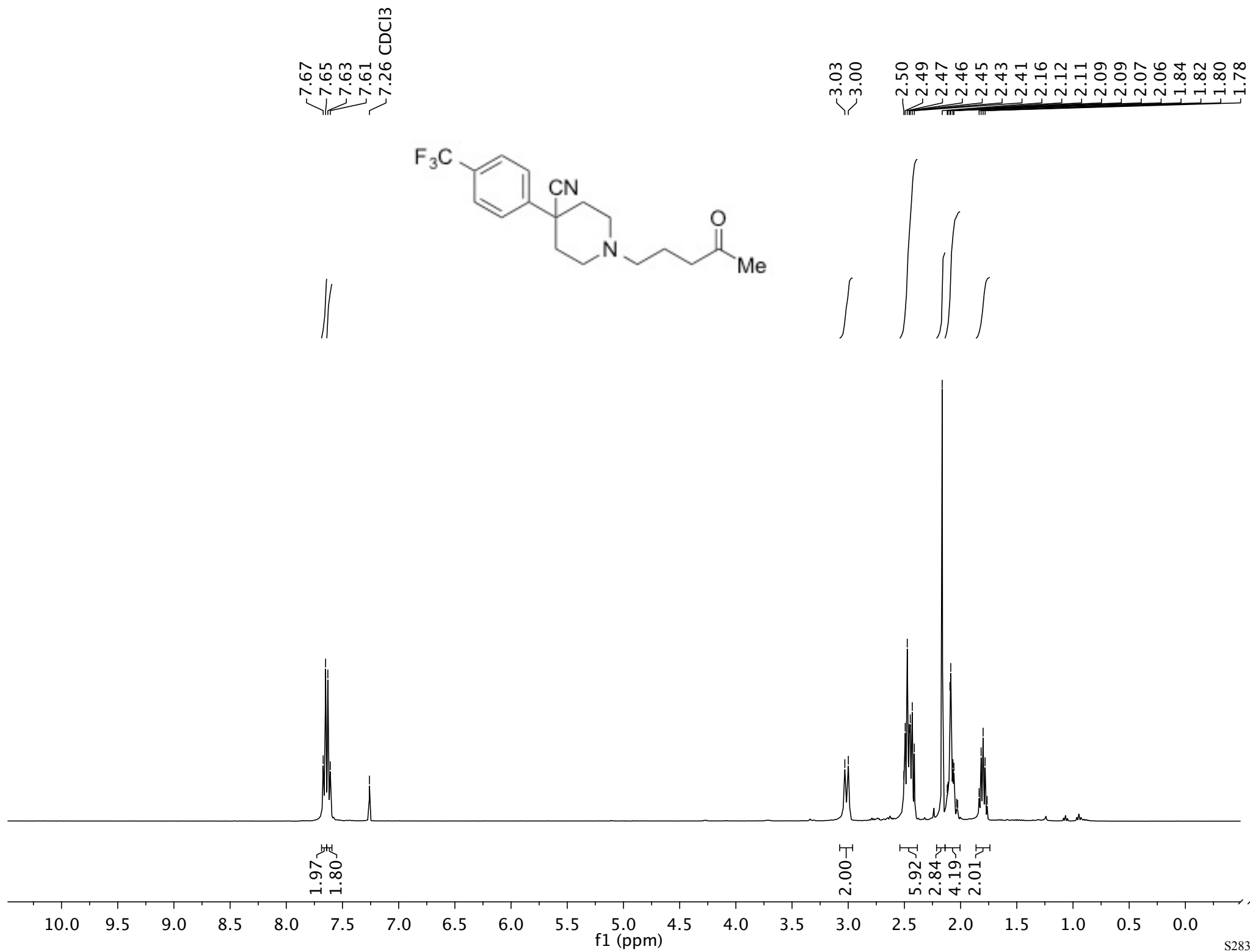
63.24

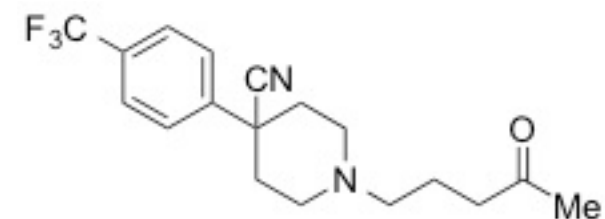
3.00

f1 (ppm)

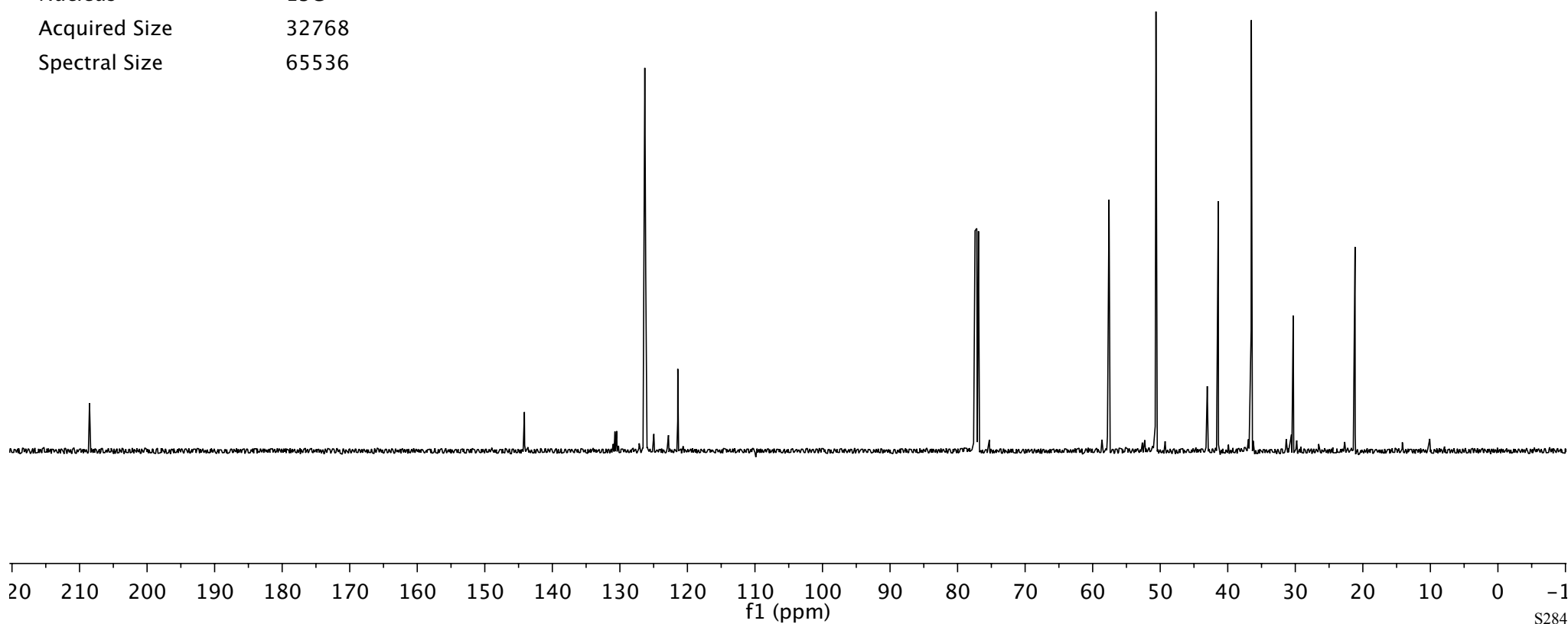
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	46
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	399.95
Spectral Width	8000.0
Lowest Frequency	-2424.5
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

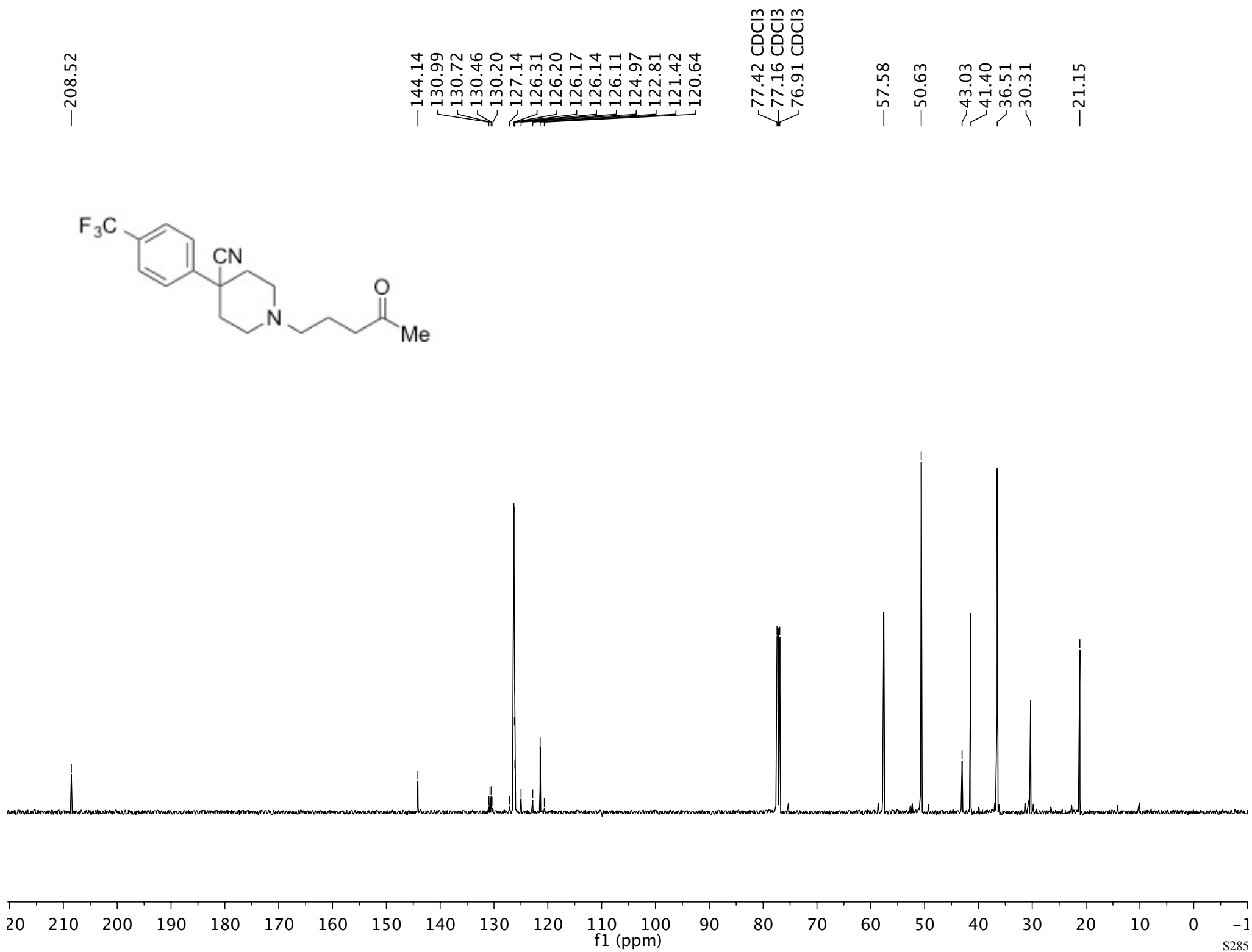




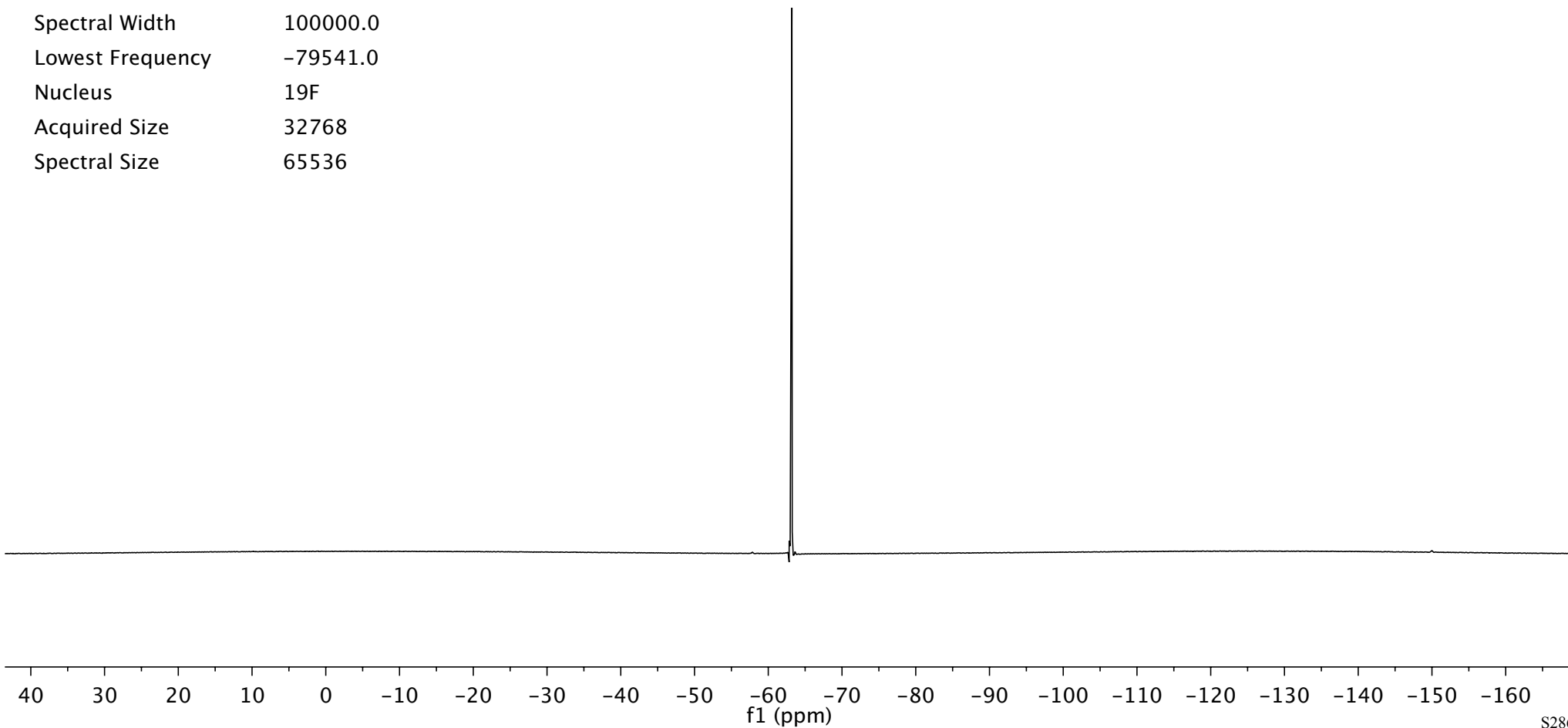
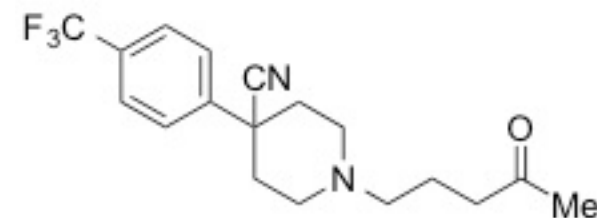


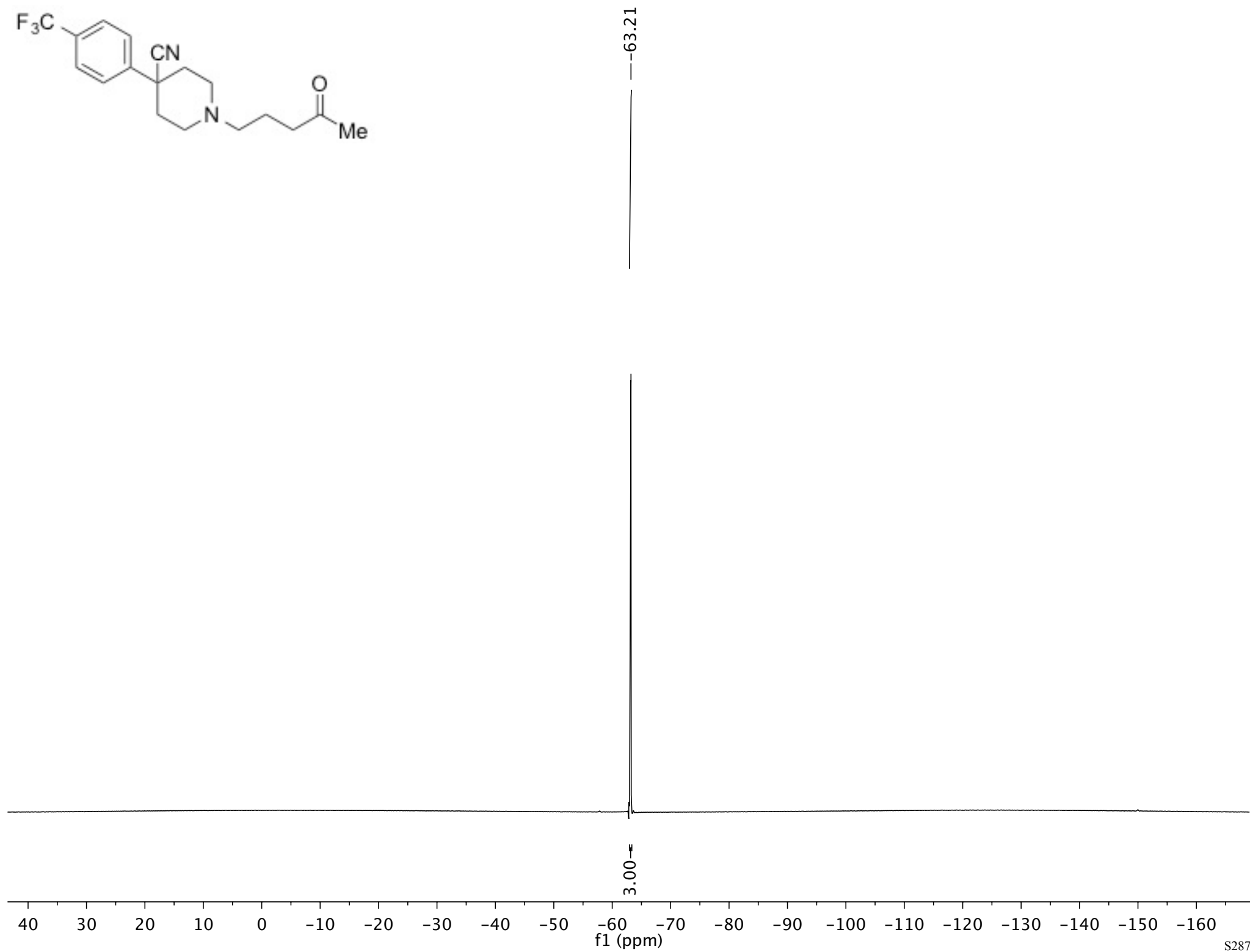
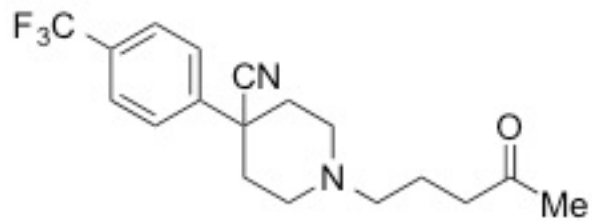
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1275.8
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



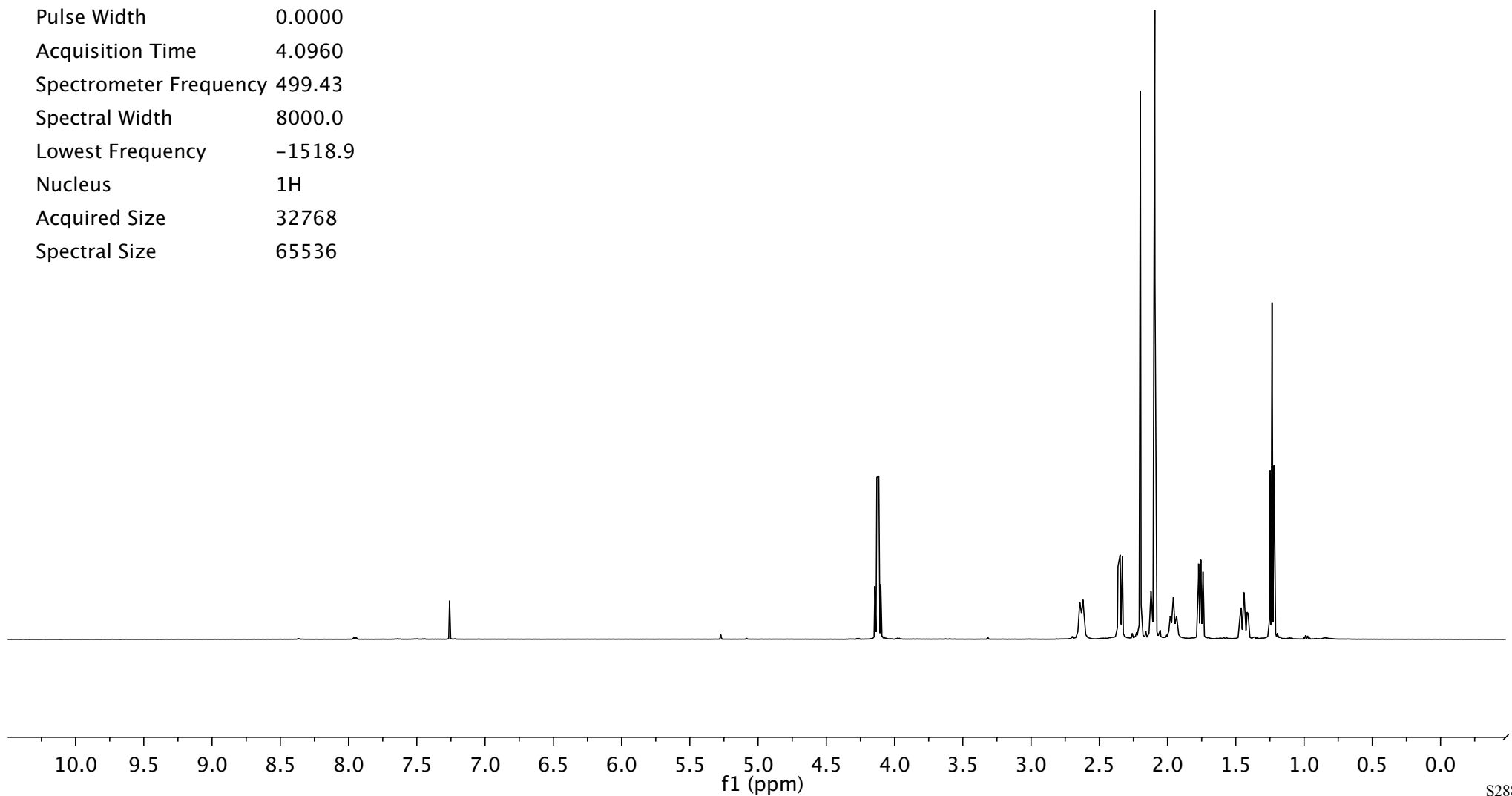
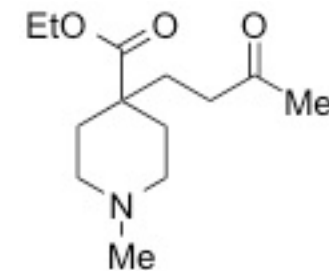


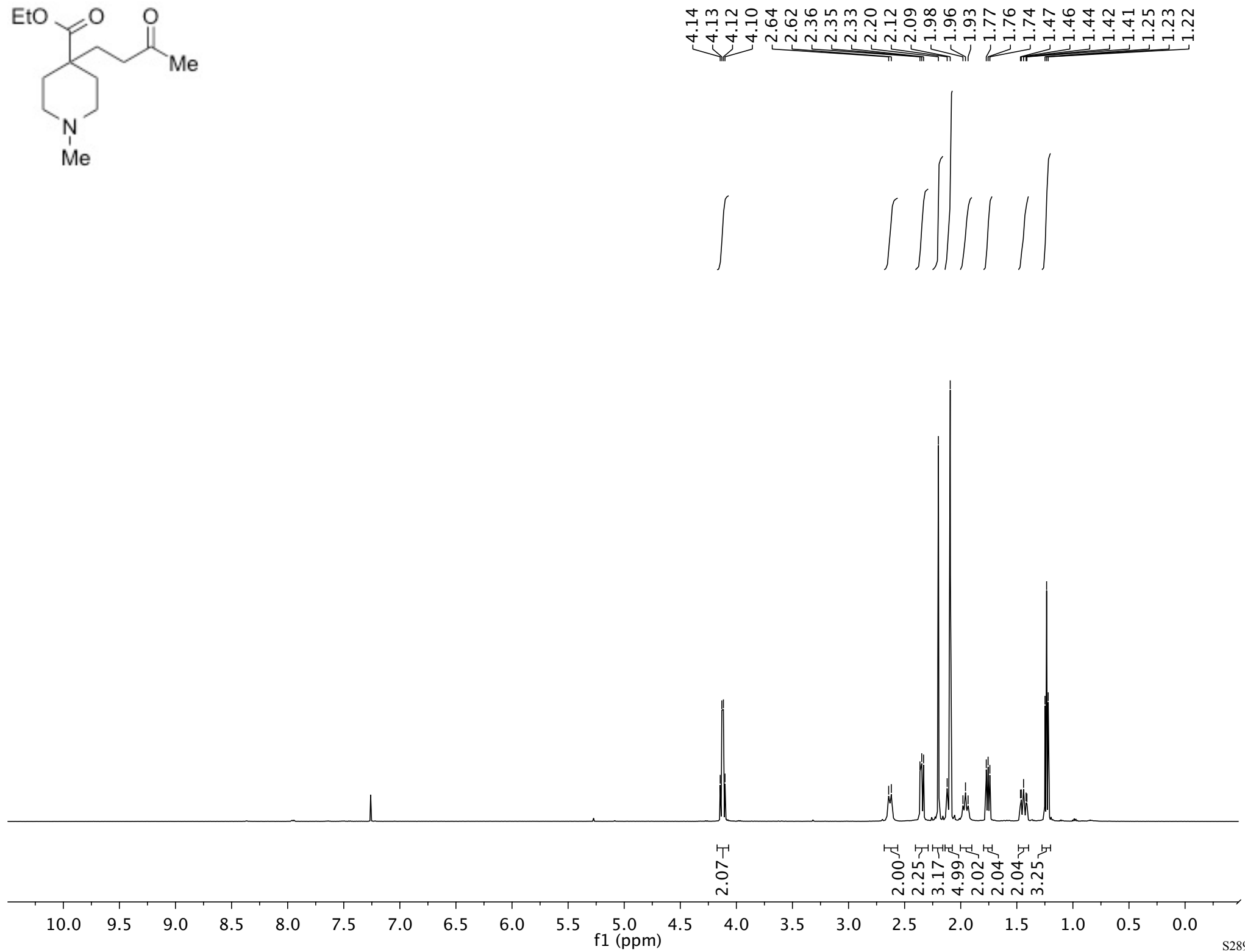
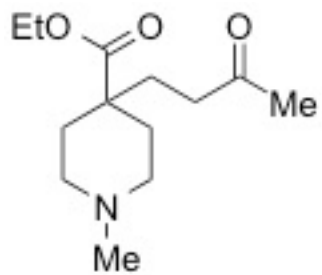
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	50
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency	-79541.0
Nucleus	¹⁹ F
Acquired Size	32768
Spectral Size	65536



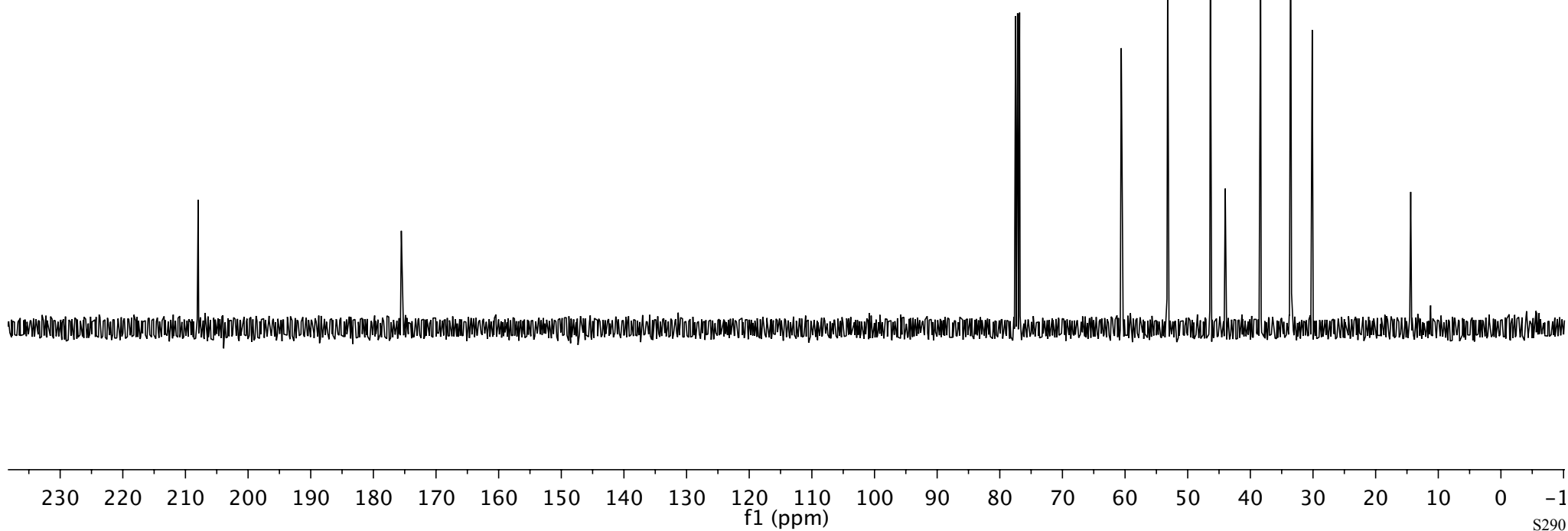
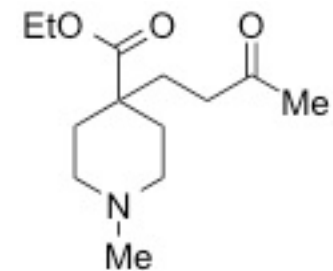


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	44
Relaxation Delay	5.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	499.43
Spectral Width	8000.0
Lowest Frequency	-1518.9
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



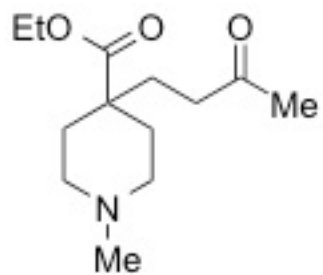


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.3107
Spectrometer Frequency	100.58
Spectral Width	25000.0
Lowest Frequency	-1028.1
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



—207.97

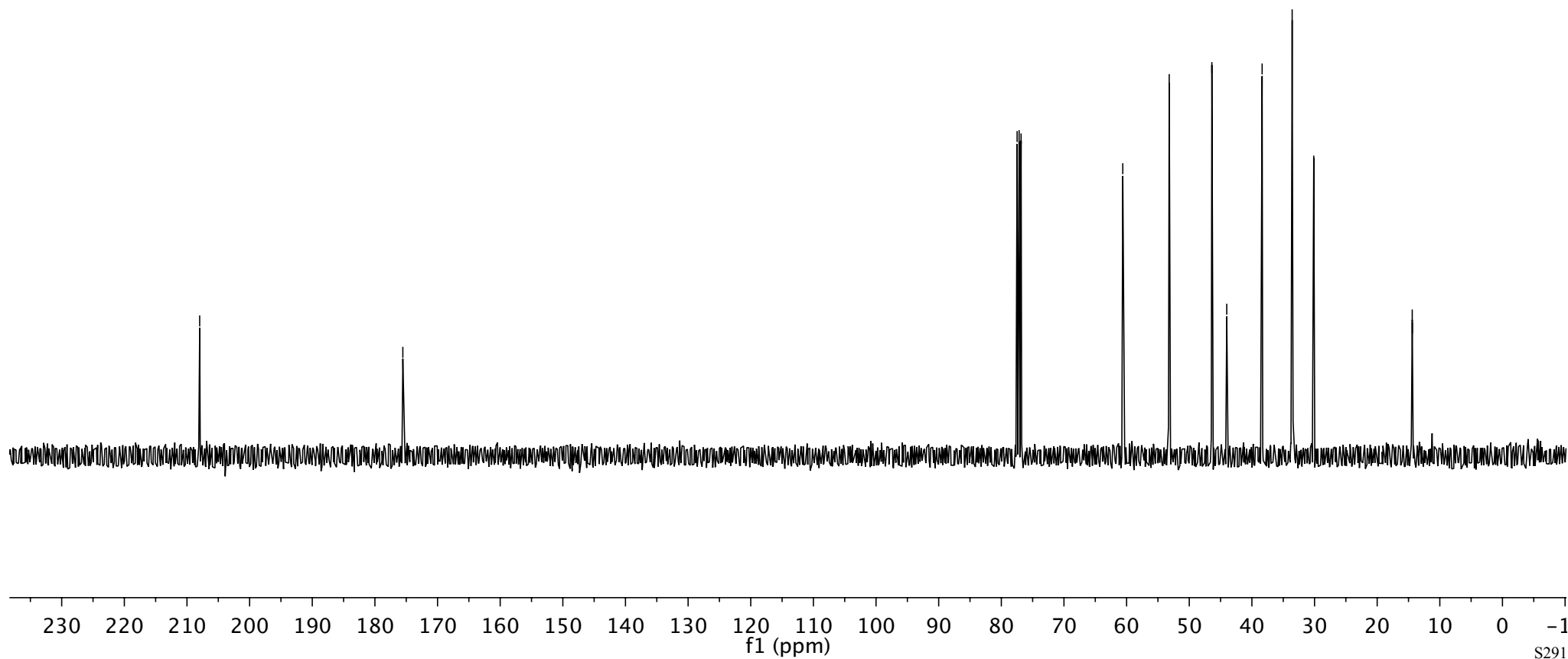
—175.54



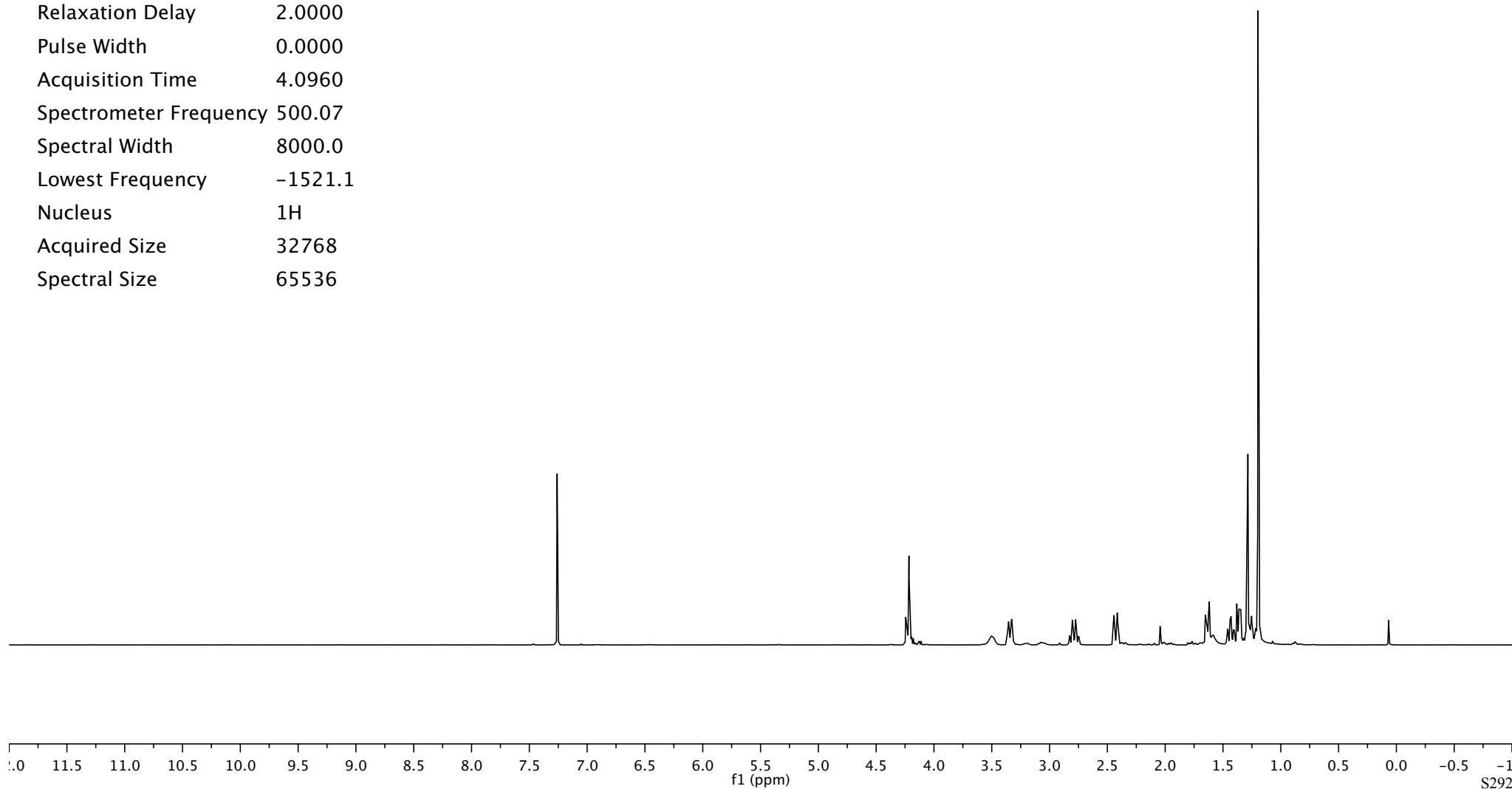
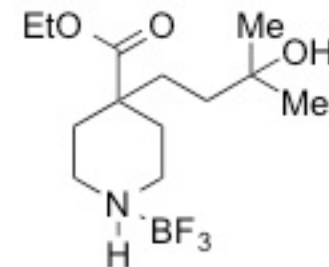
77.48 CDCl₃
77.16 CDCl₃
76.84 CDCl₃

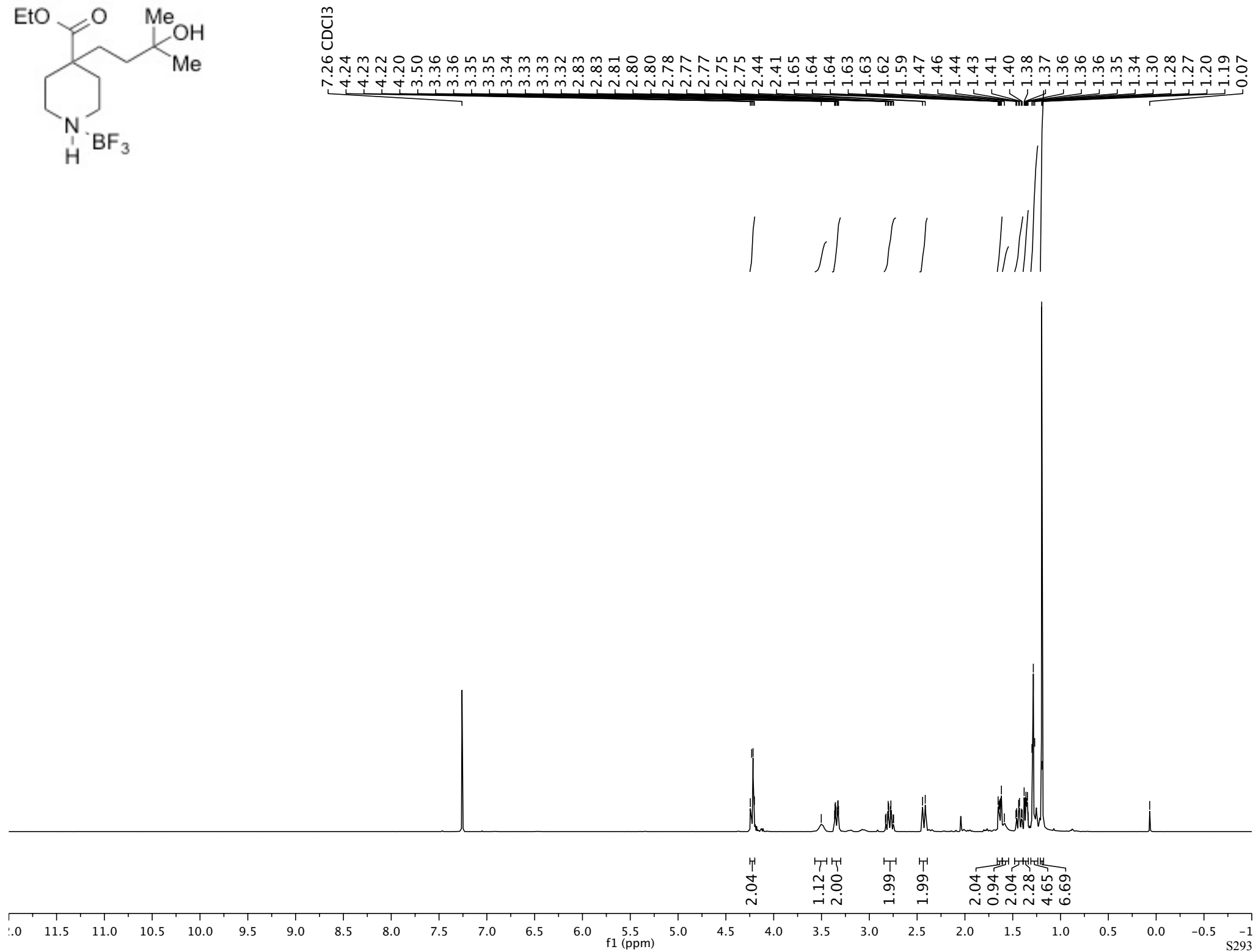
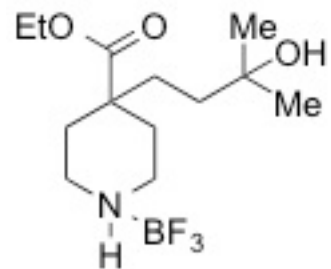
60.61
53.20
46.39
44.01
38.36
33.57
30.12

14.40
14.38

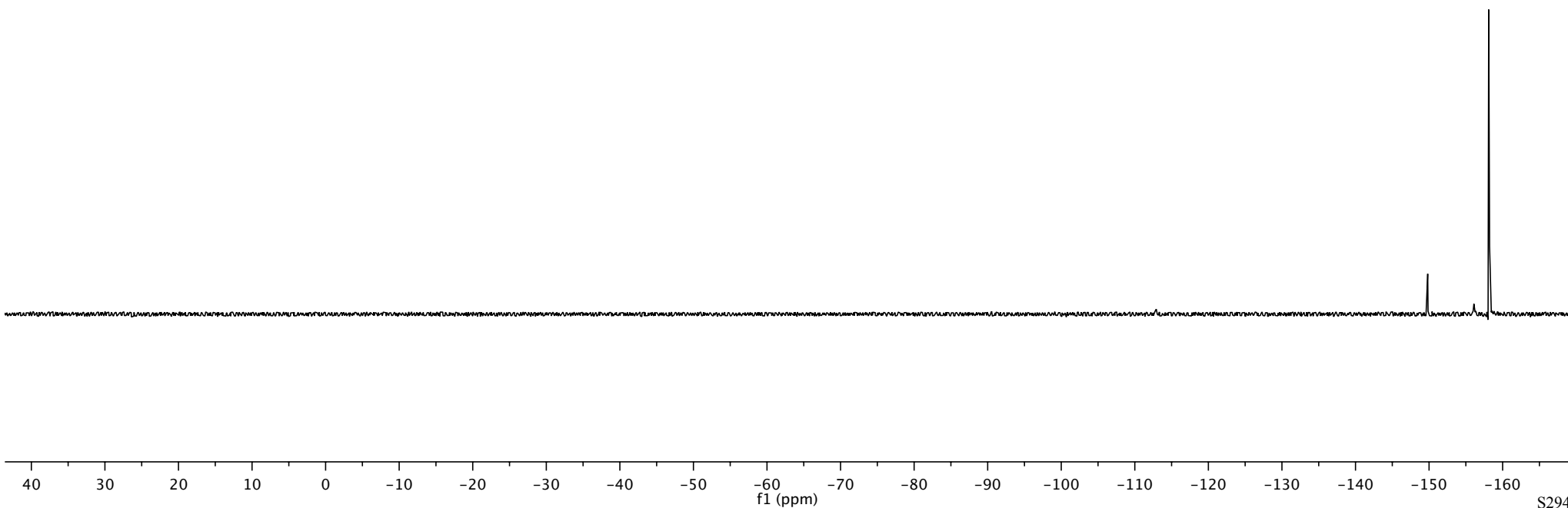
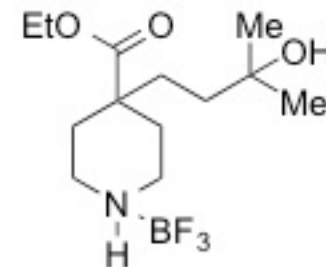


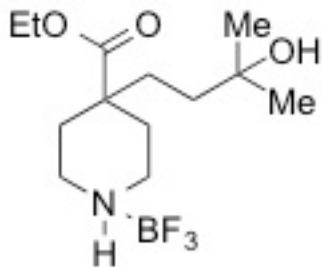
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	44
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	^1H
Acquired Size	32768
Spectral Size	65536



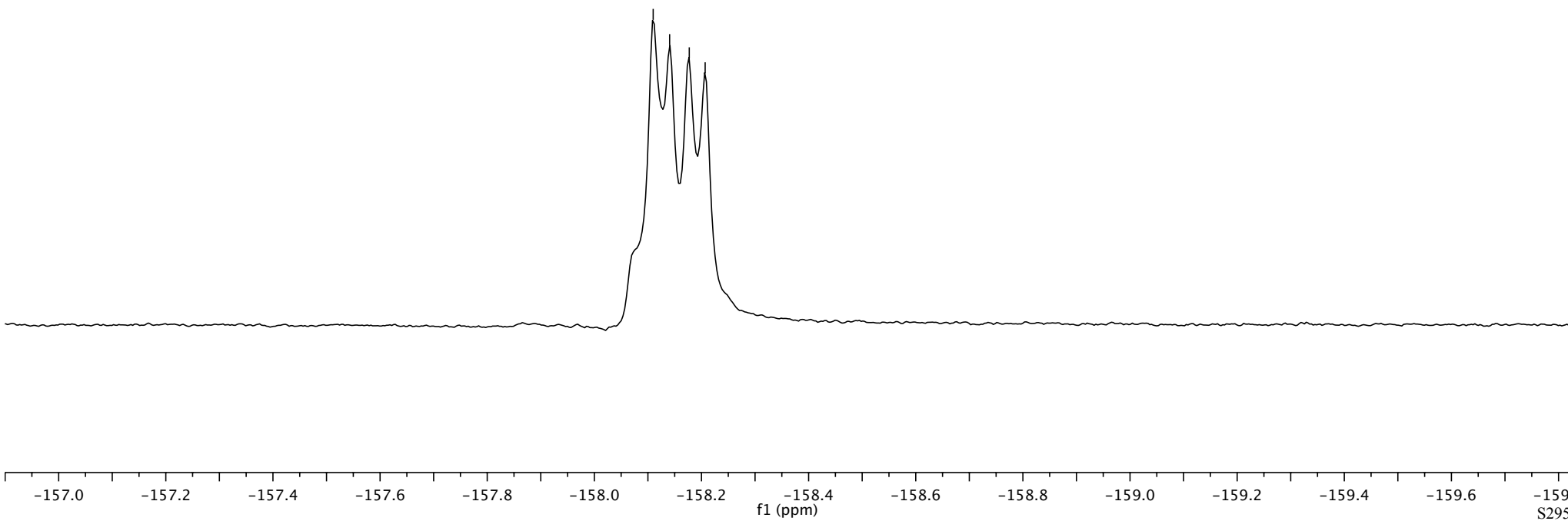


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	22.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	64
Receiver Gain	50
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency	-79501.3
Nucleus	¹⁹ F
Acquired Size	32768
Spectral Size	65536

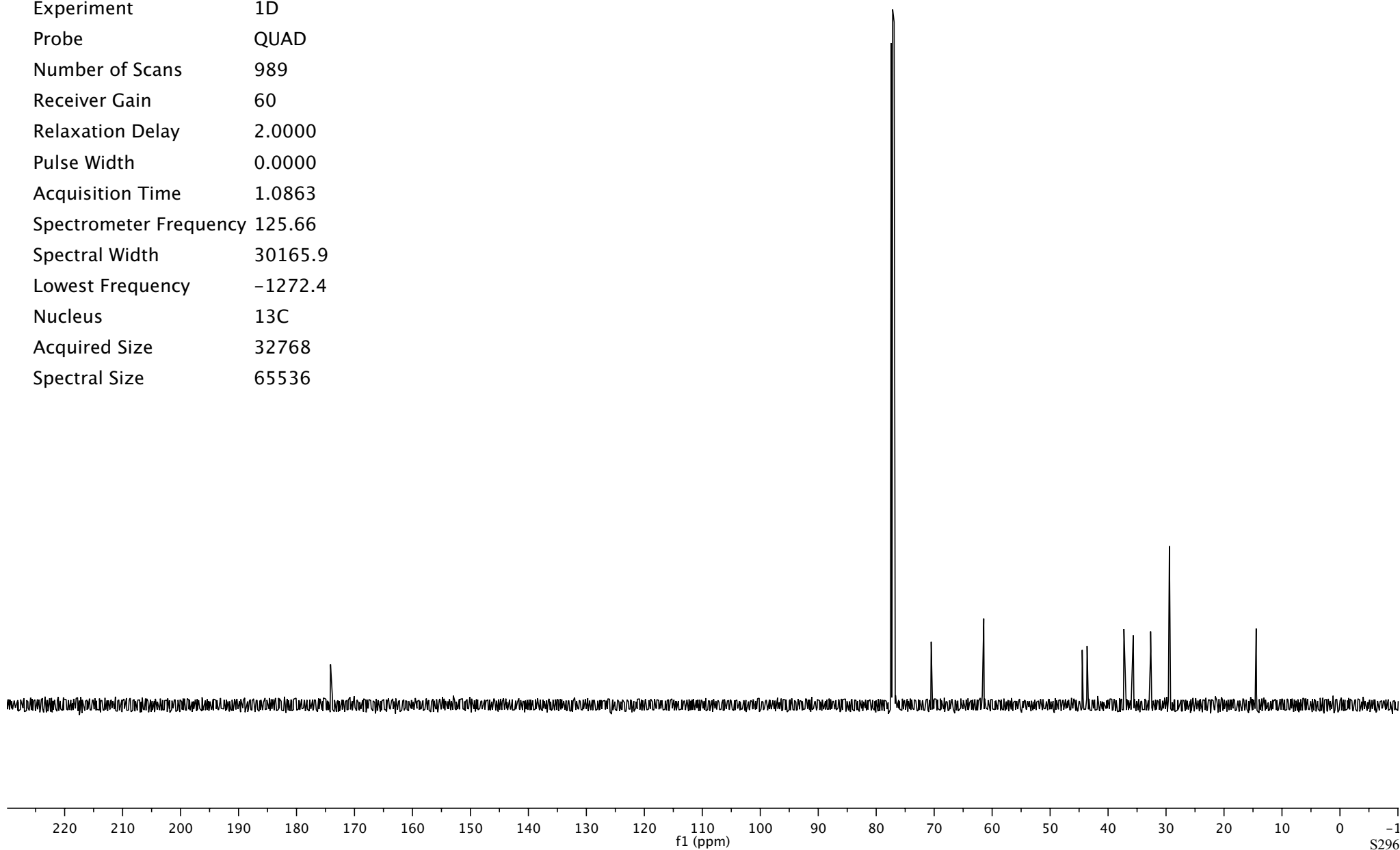
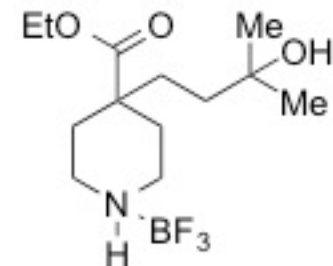


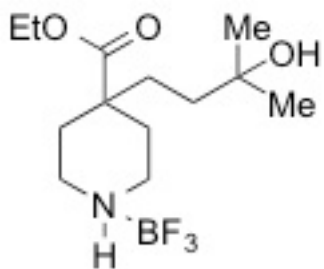


~158.11
~158.14
~158.18
~158.21



Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	22.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	989
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1272.4
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536





—174.13

—77.16 CDCl₃

—70.52

—61.45

—44.46

—43.63

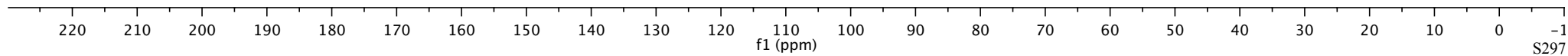
—37.27

—35.67

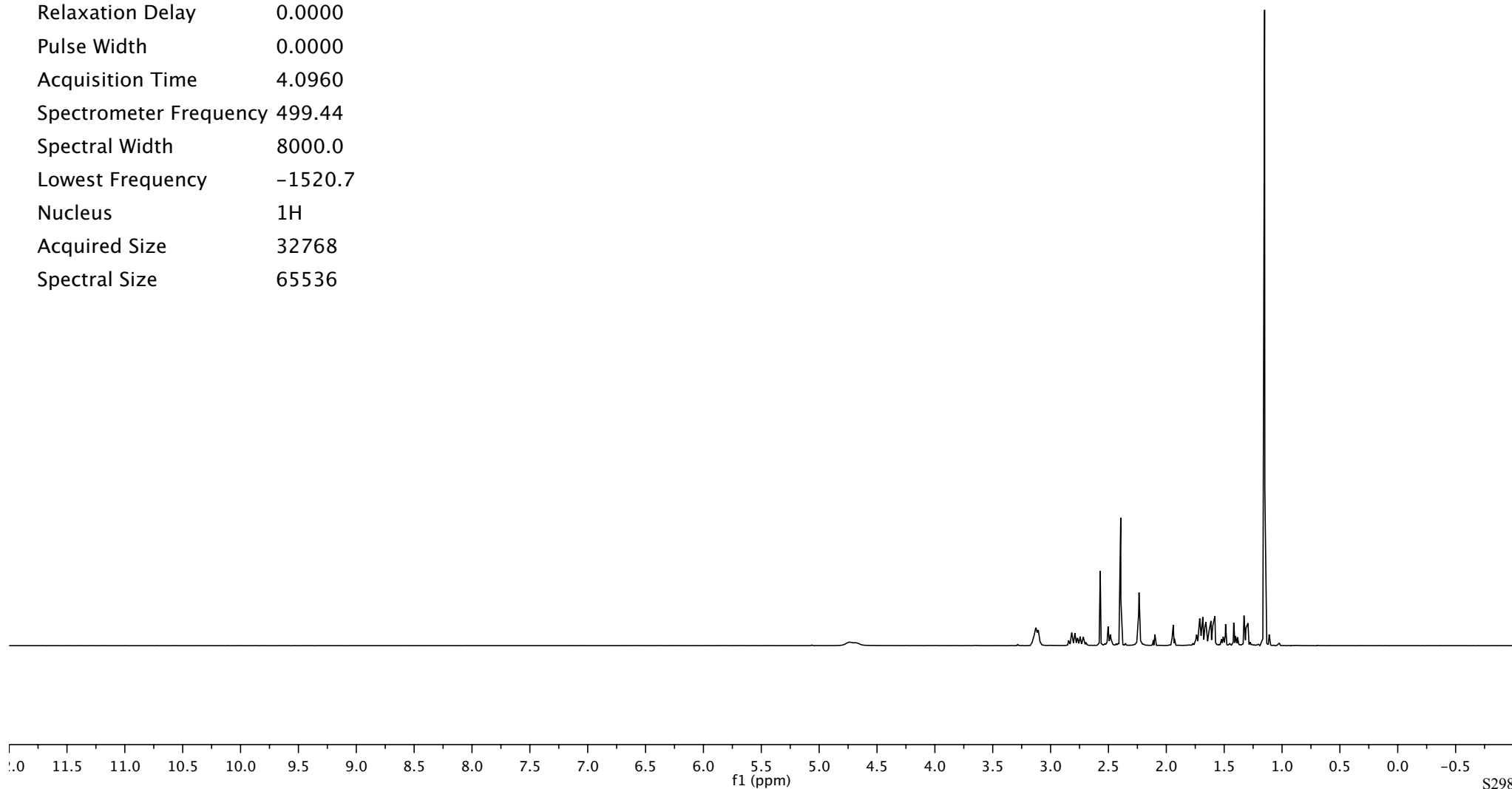
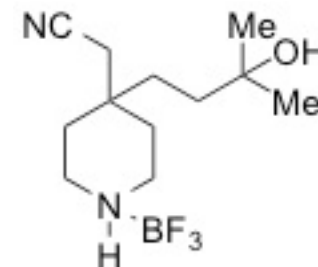
—32.66

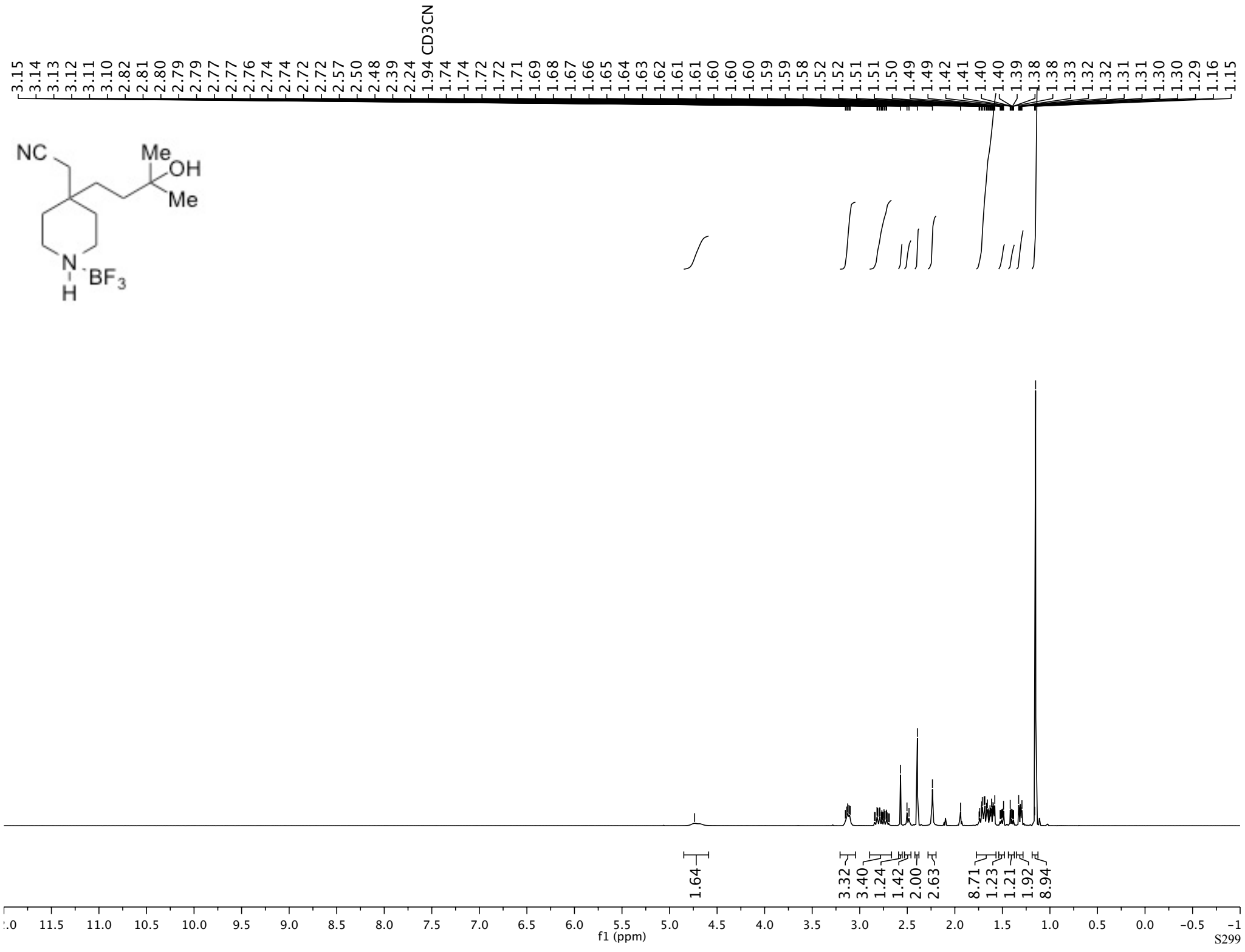
—29.42

—14.45

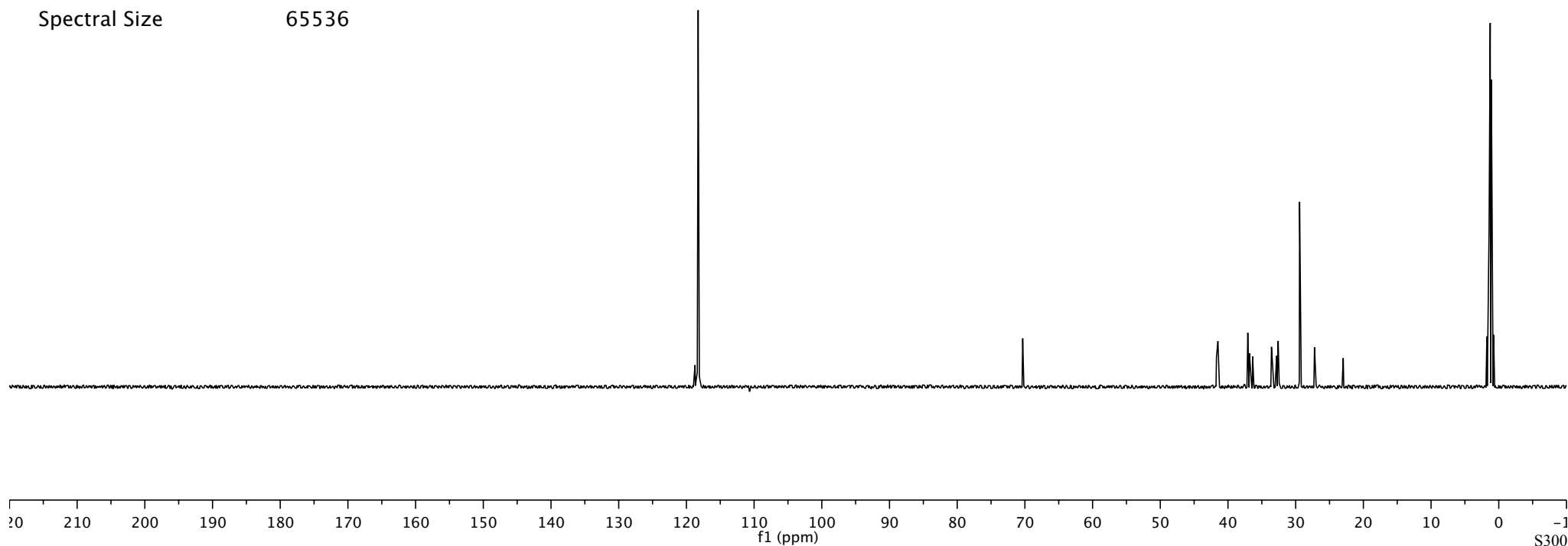
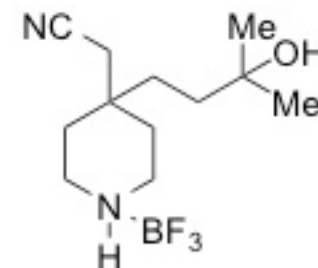


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CD ₃ CN
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Number of Scans	8
Receiver Gain	44
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	499.44
Spectral Width	8000.0
Lowest Frequency	-1520.7
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

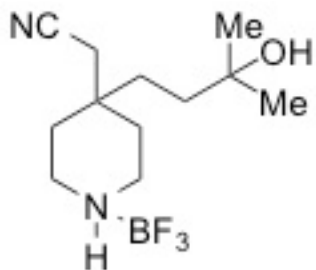




Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CD ₃ CN
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Number of Scans	928
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2100.4
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

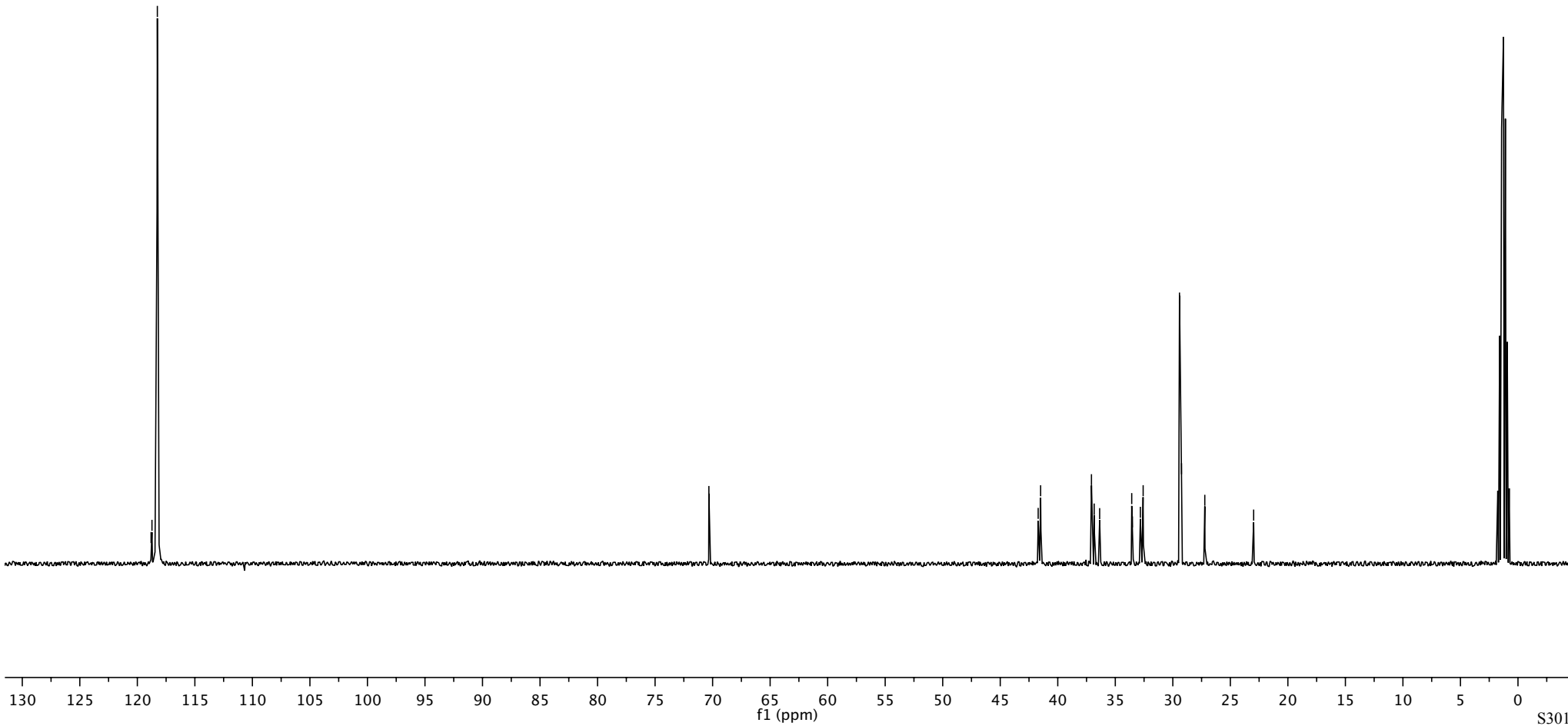


118.81
118.73
118.26 CD₃CN

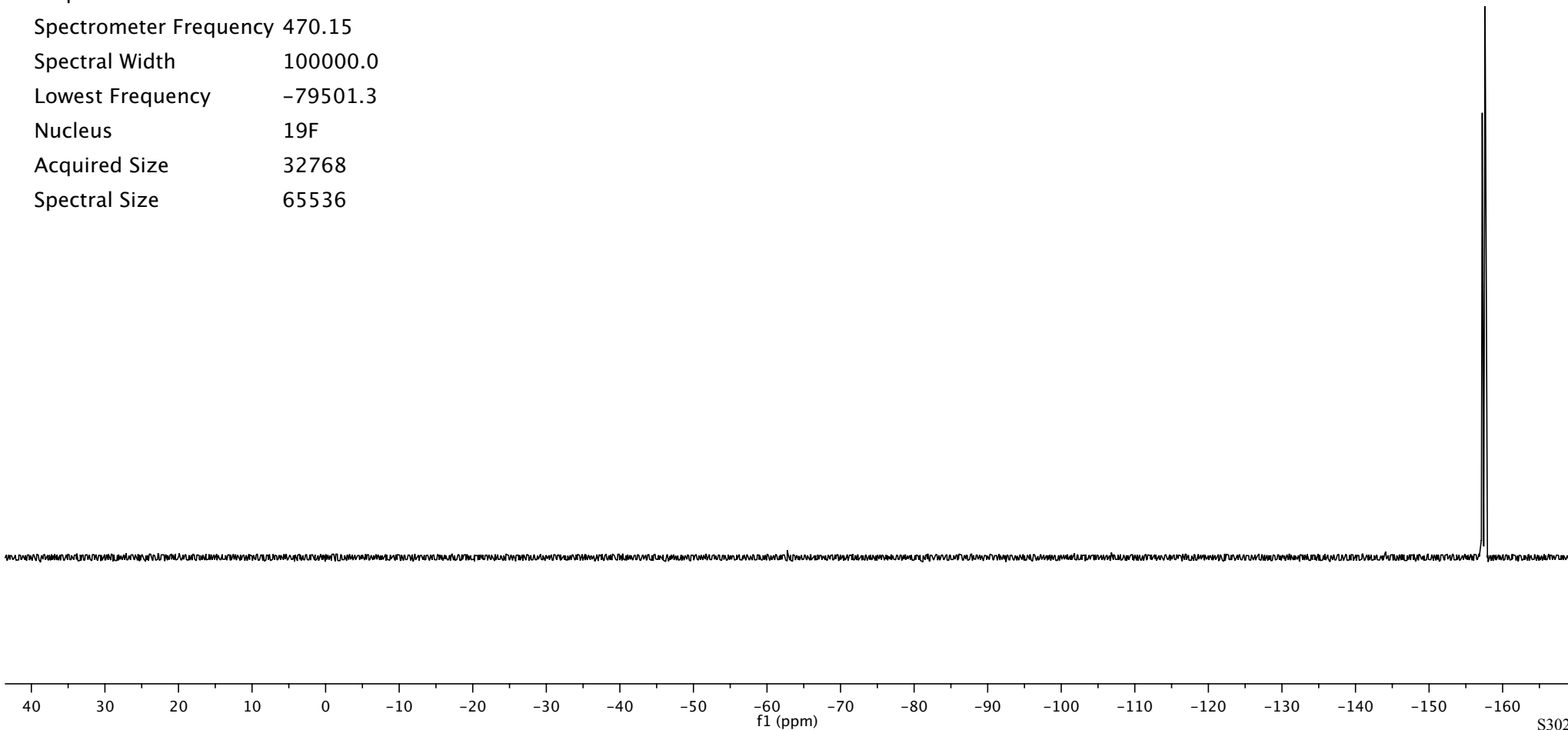
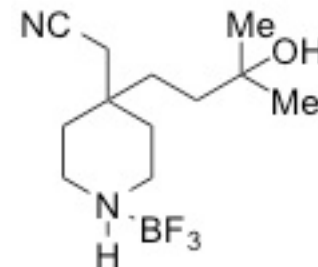


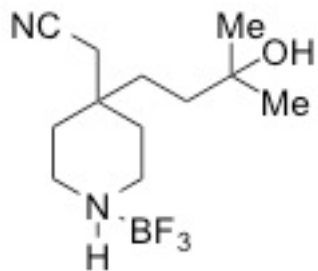
70.32
70.30

41.70
41.49
37.07
36.83
36.36
33.57
33.51
32.82
32.58
29.42
29.25
27.22
-22.97



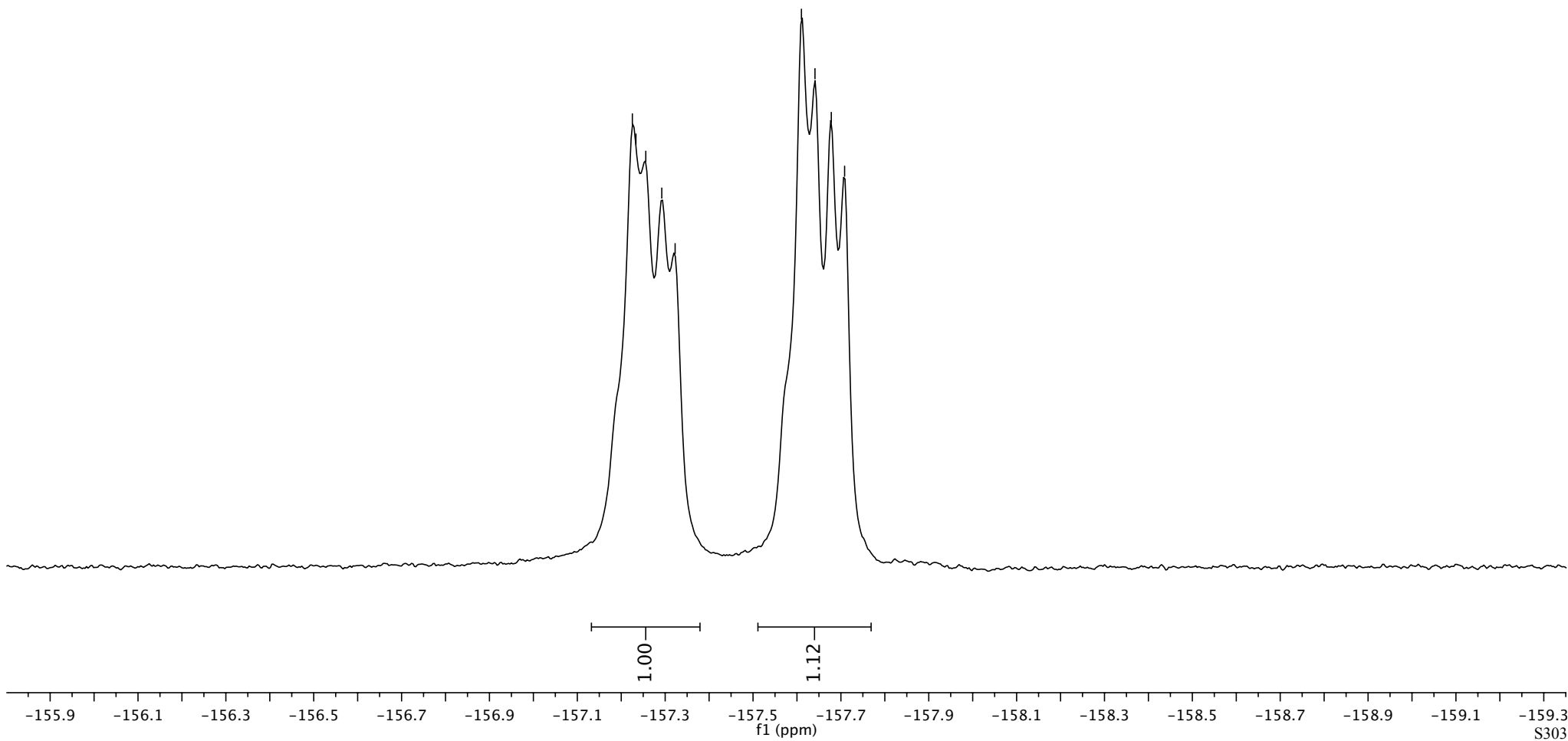
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	64
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency	-79501.3
Nucleus	¹⁹ F
Acquired Size	32768
Spectral Size	65536



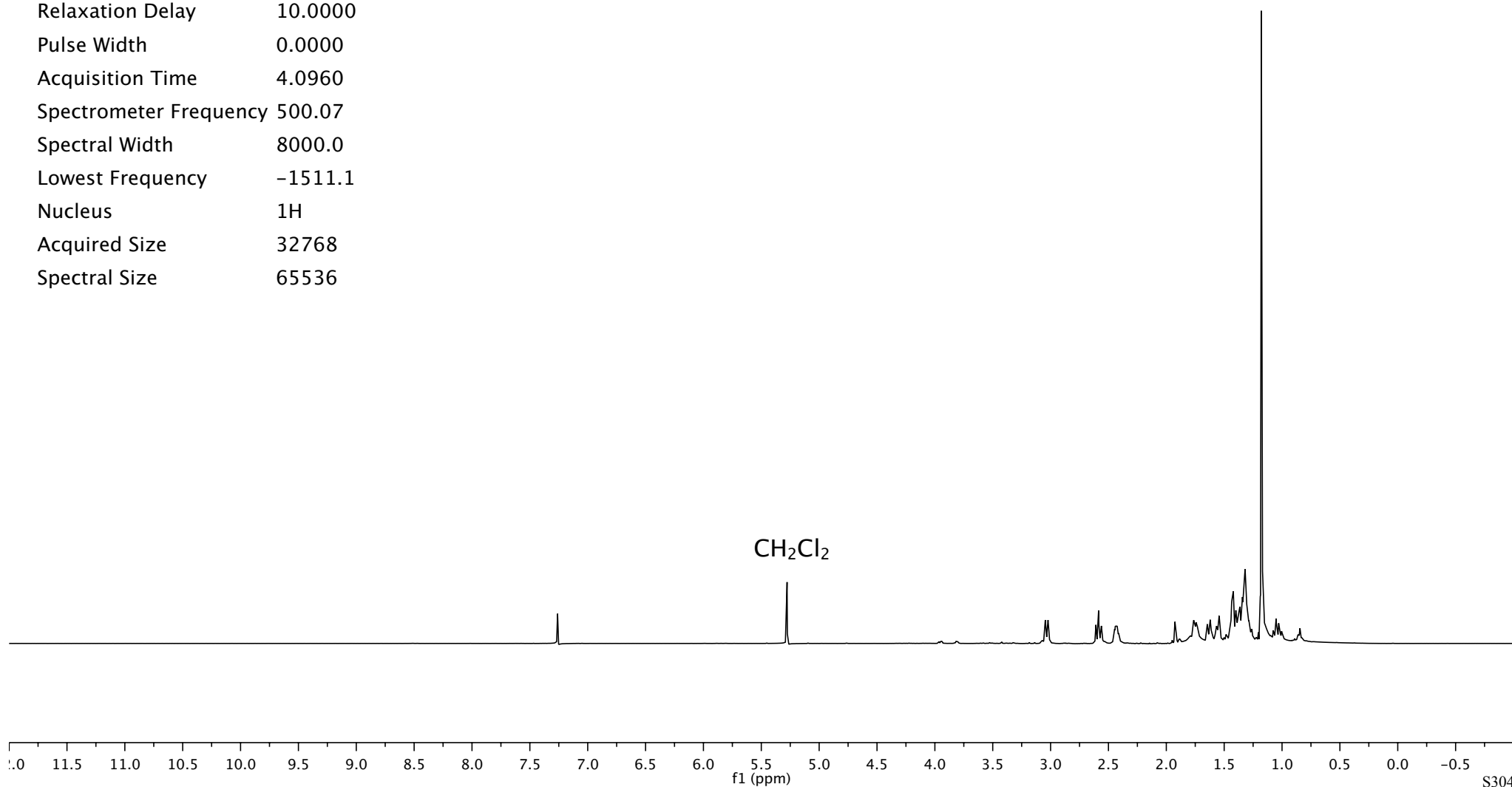
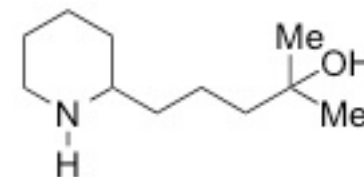


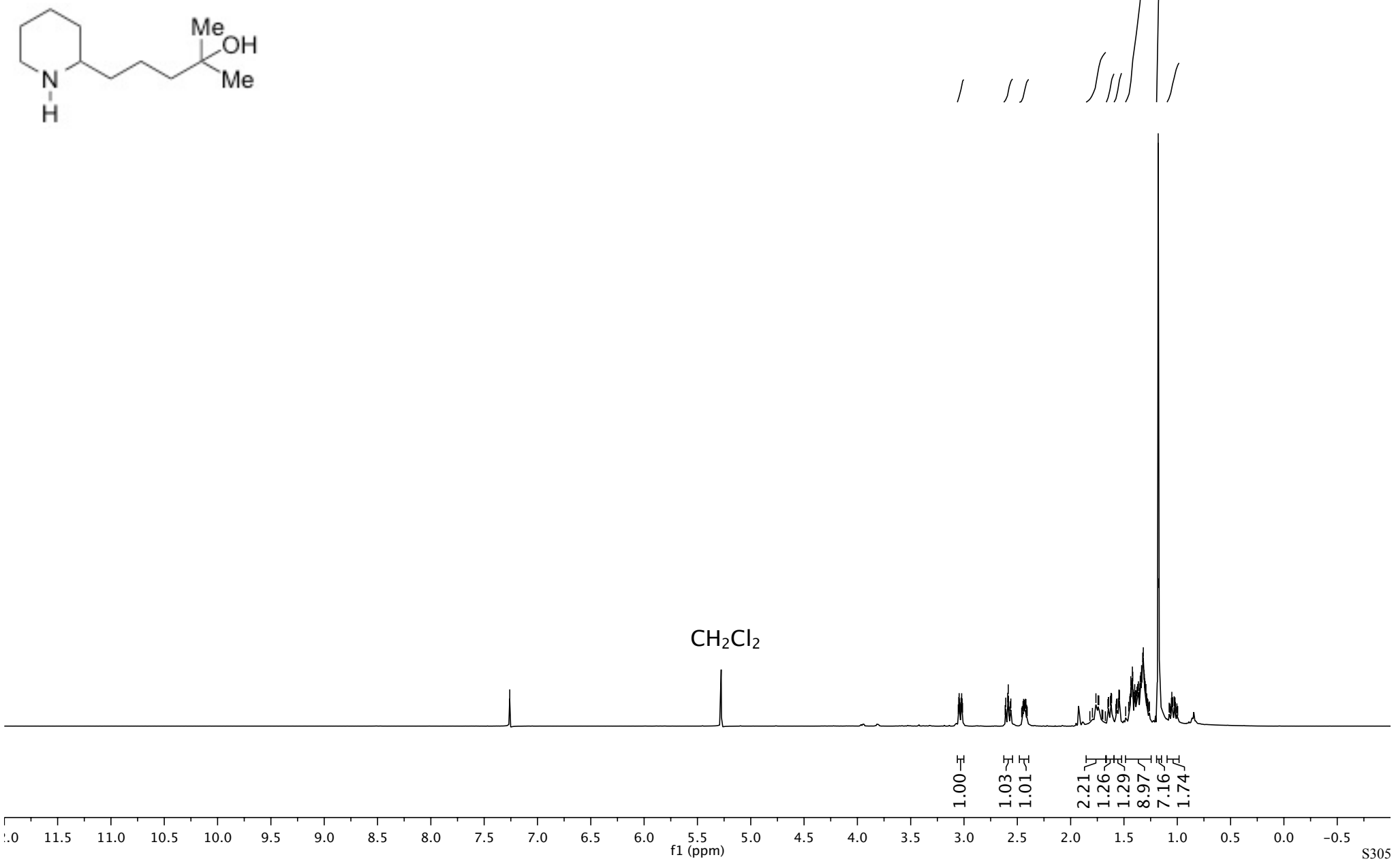
157.23
157.23
157.26
157.29
157.32

157.61
157.64
157.68
157.71

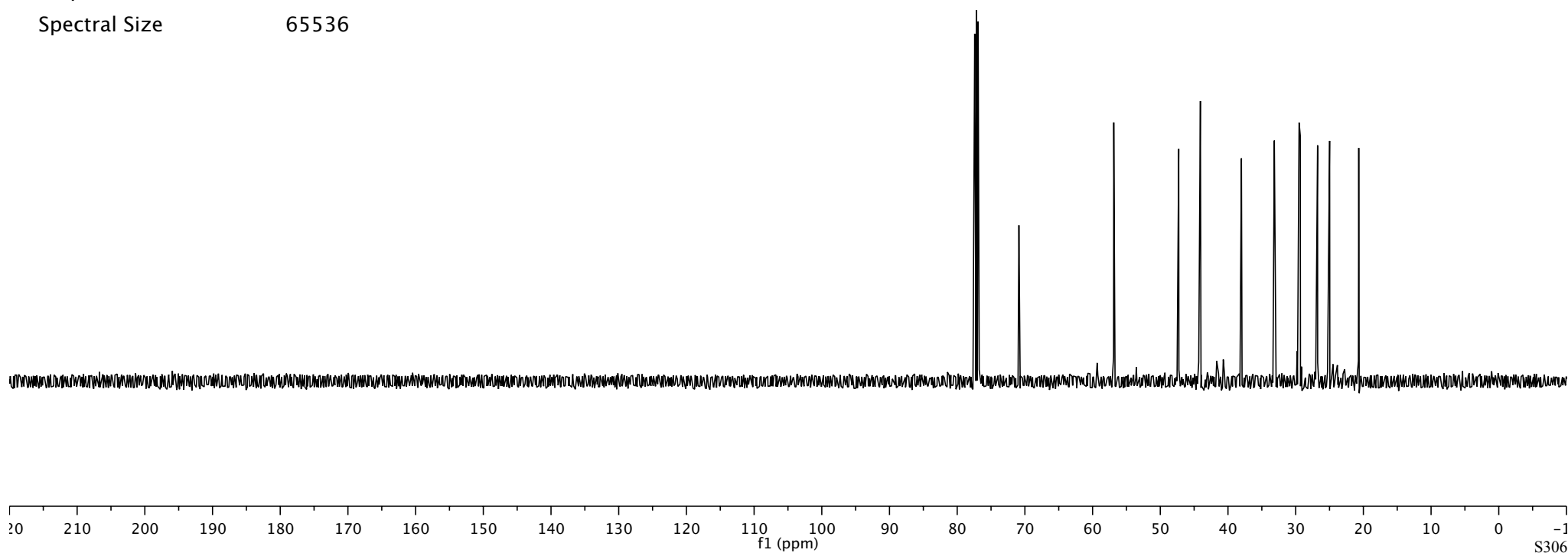
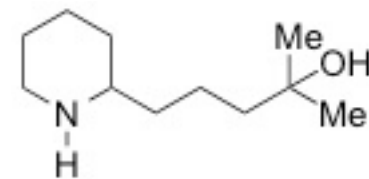


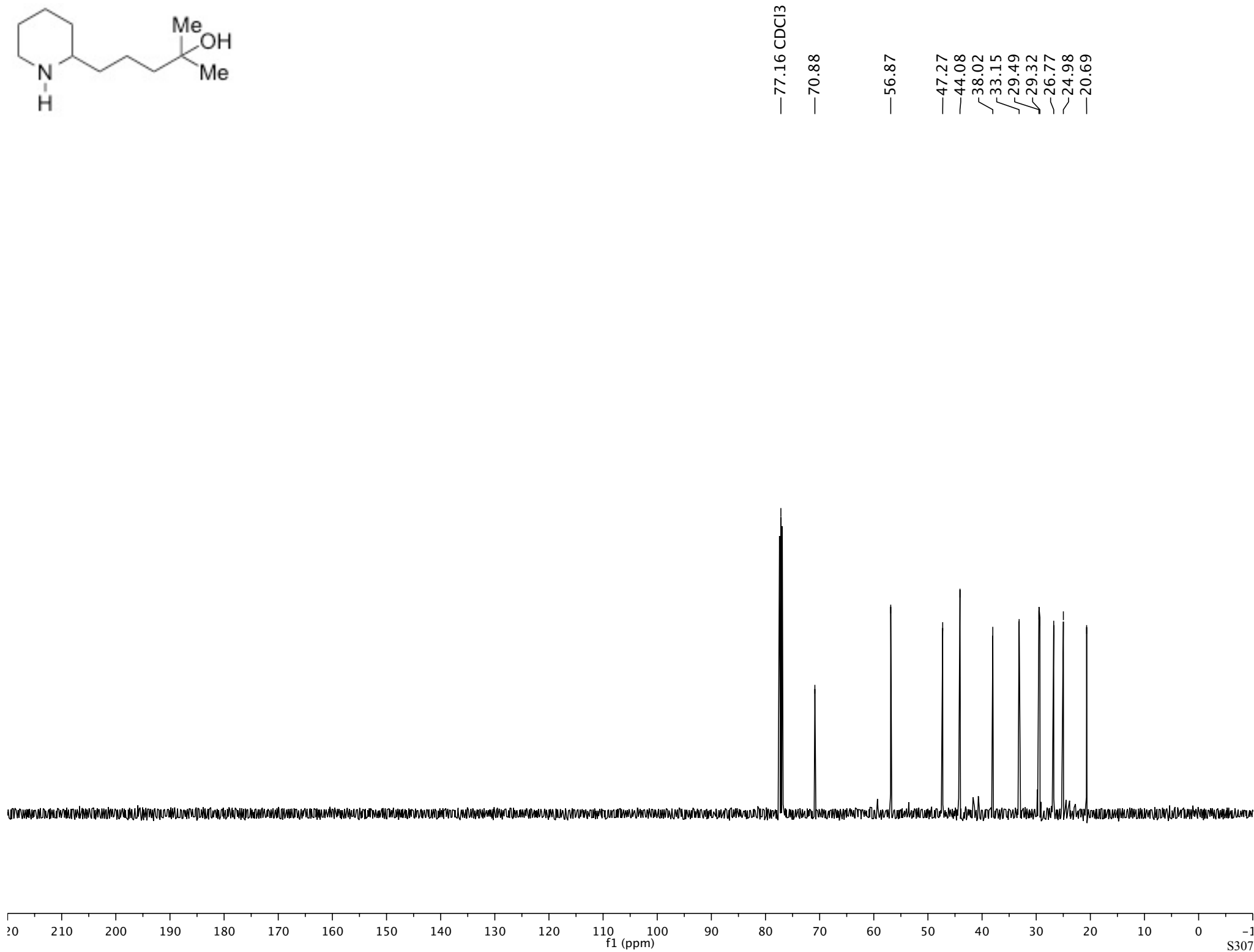
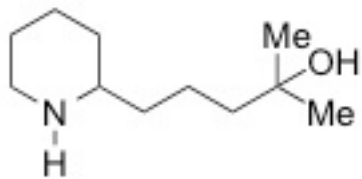
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	22
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1511.1
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



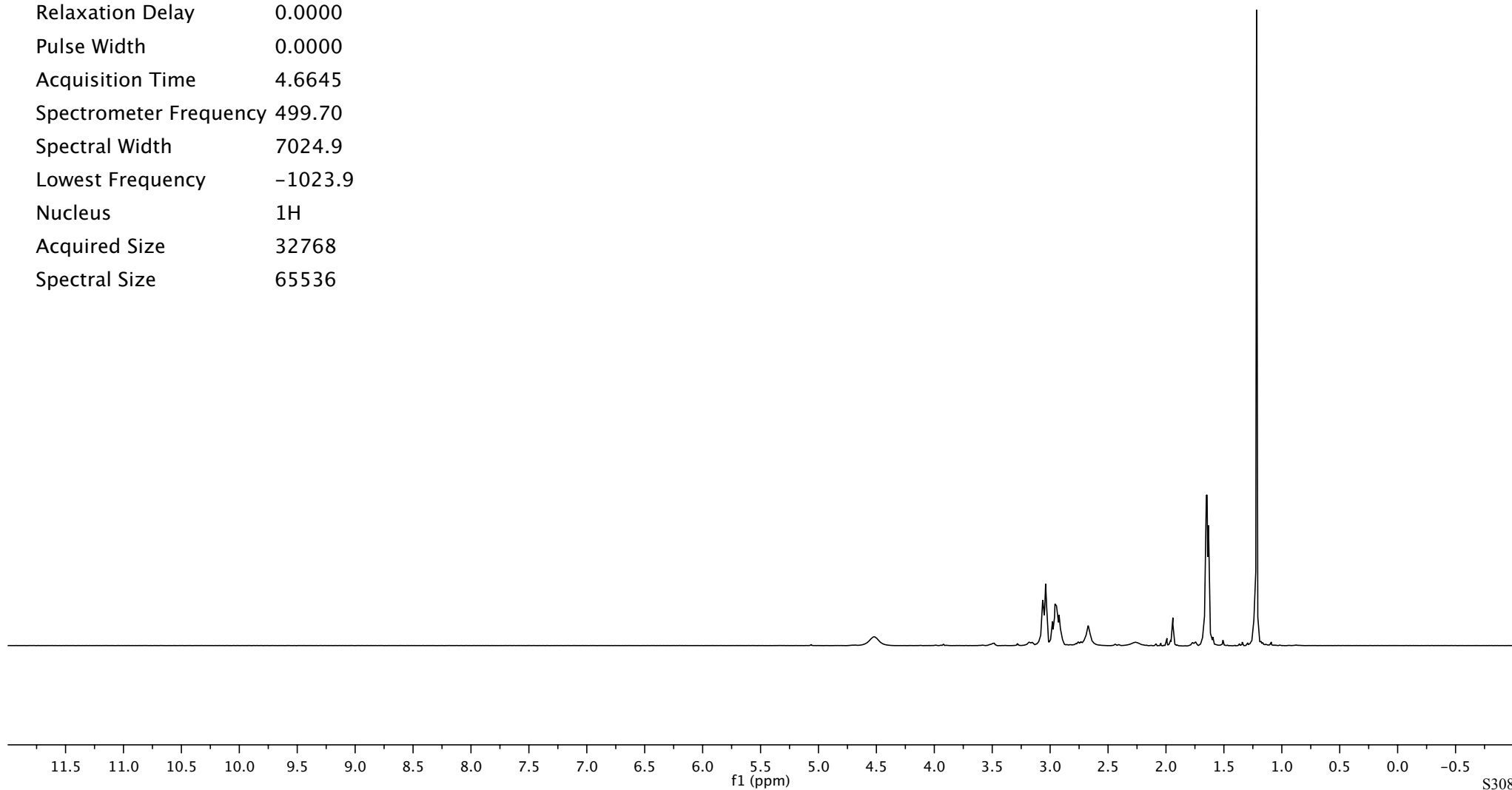
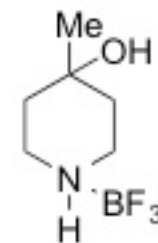


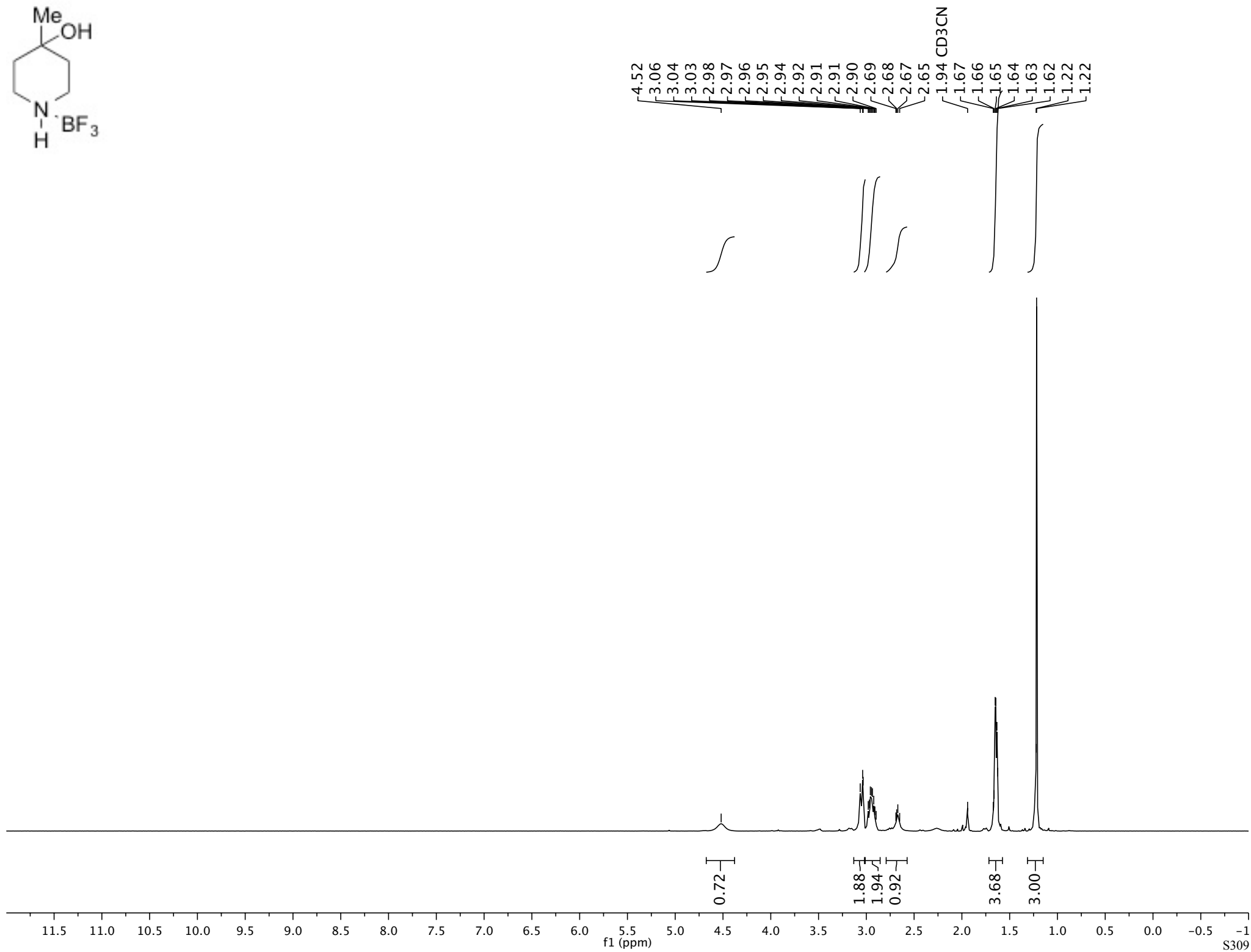
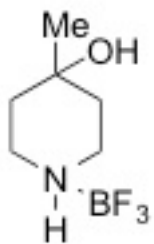
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	192
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1273.3
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



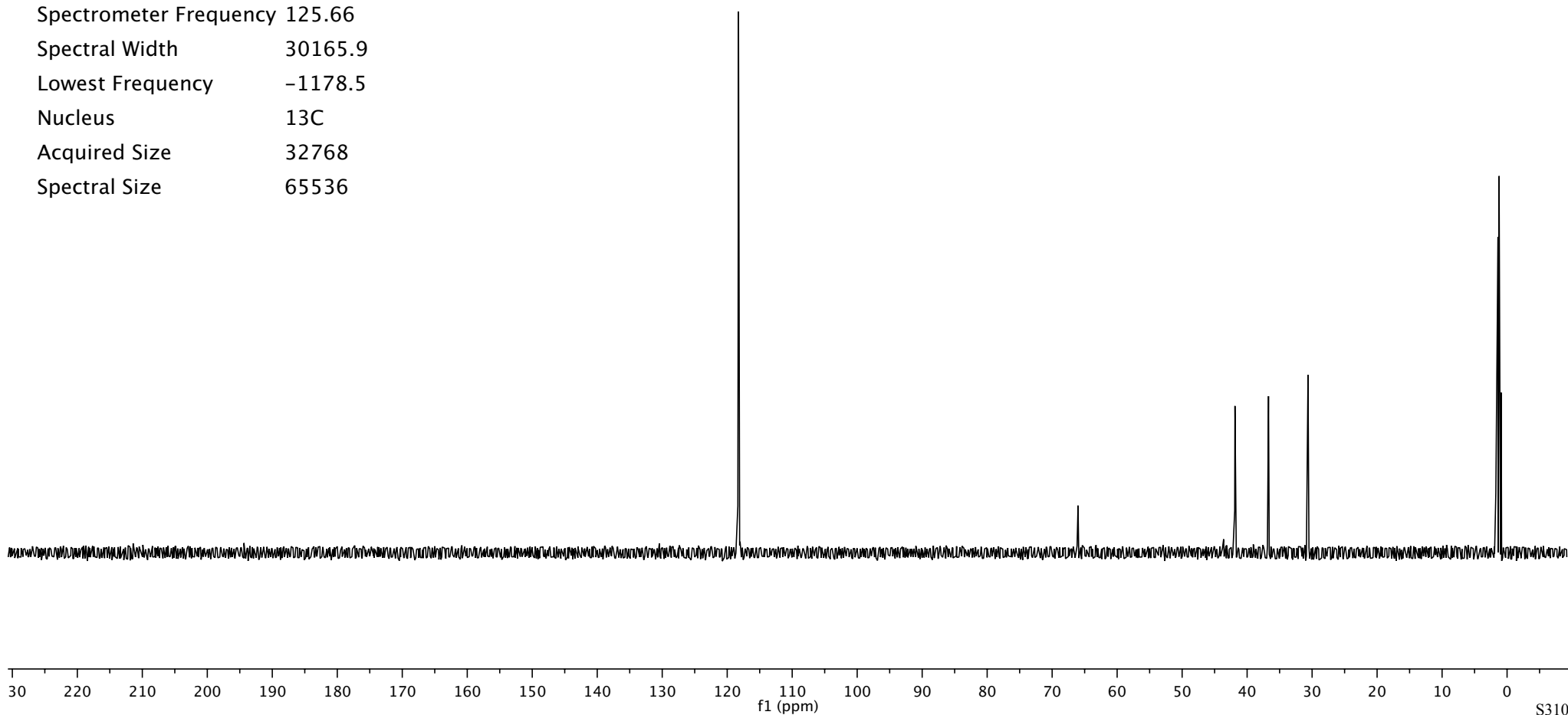
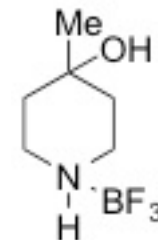


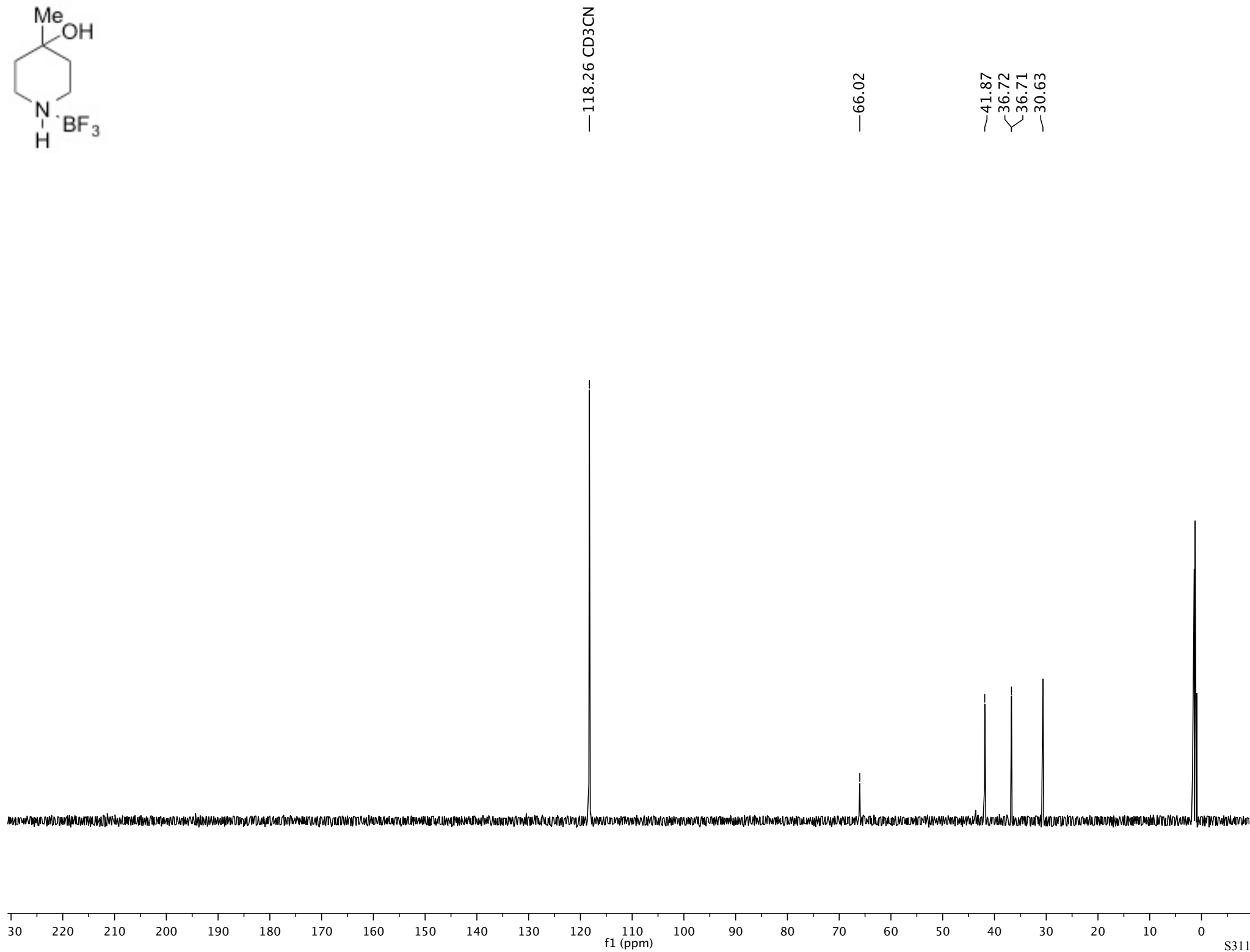
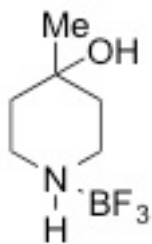
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CD3CN
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	8
Receiver Gain	41
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.70
Spectral Width	7024.9
Lowest Frequency	-1023.9
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



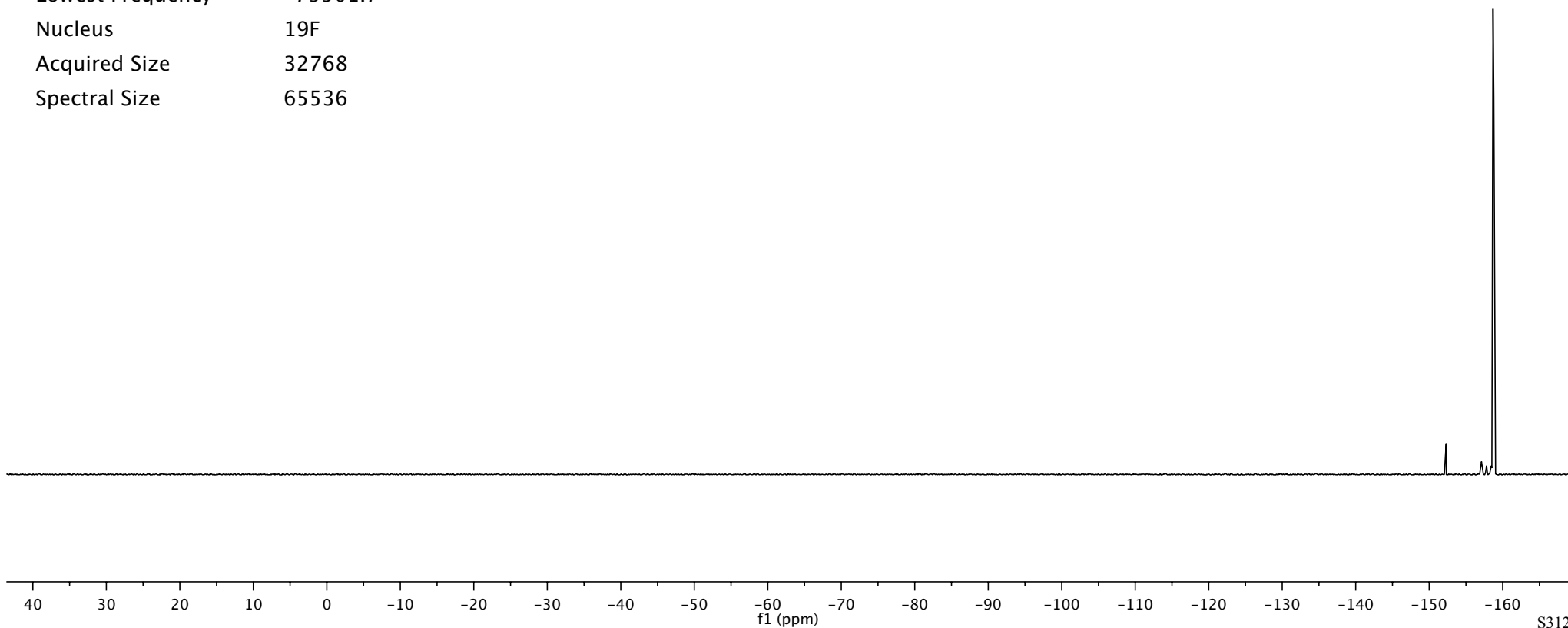
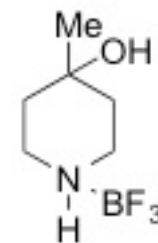


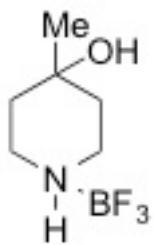
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CD3CN
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	112
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1178.5
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



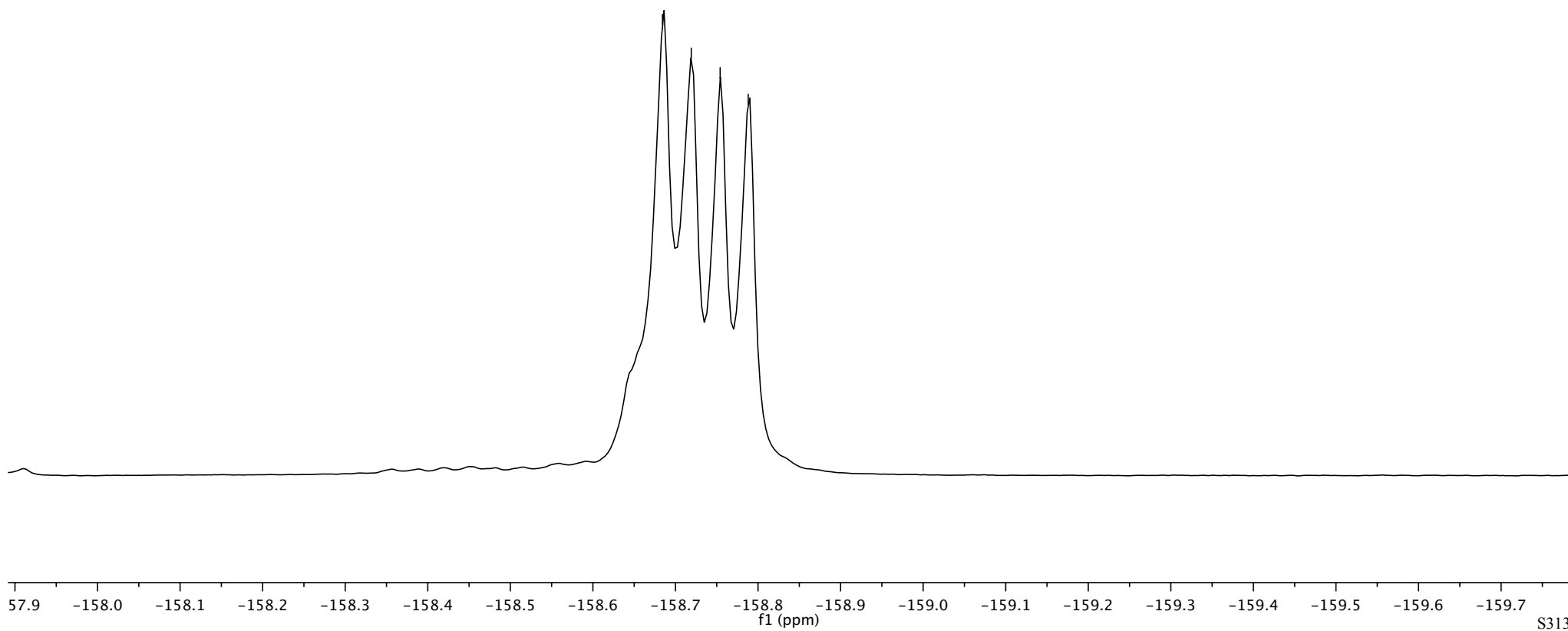


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CD3CN
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	128
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency	-79501.7
Nucleus	¹⁹ F
Acquired Size	32768
Spectral Size	65536

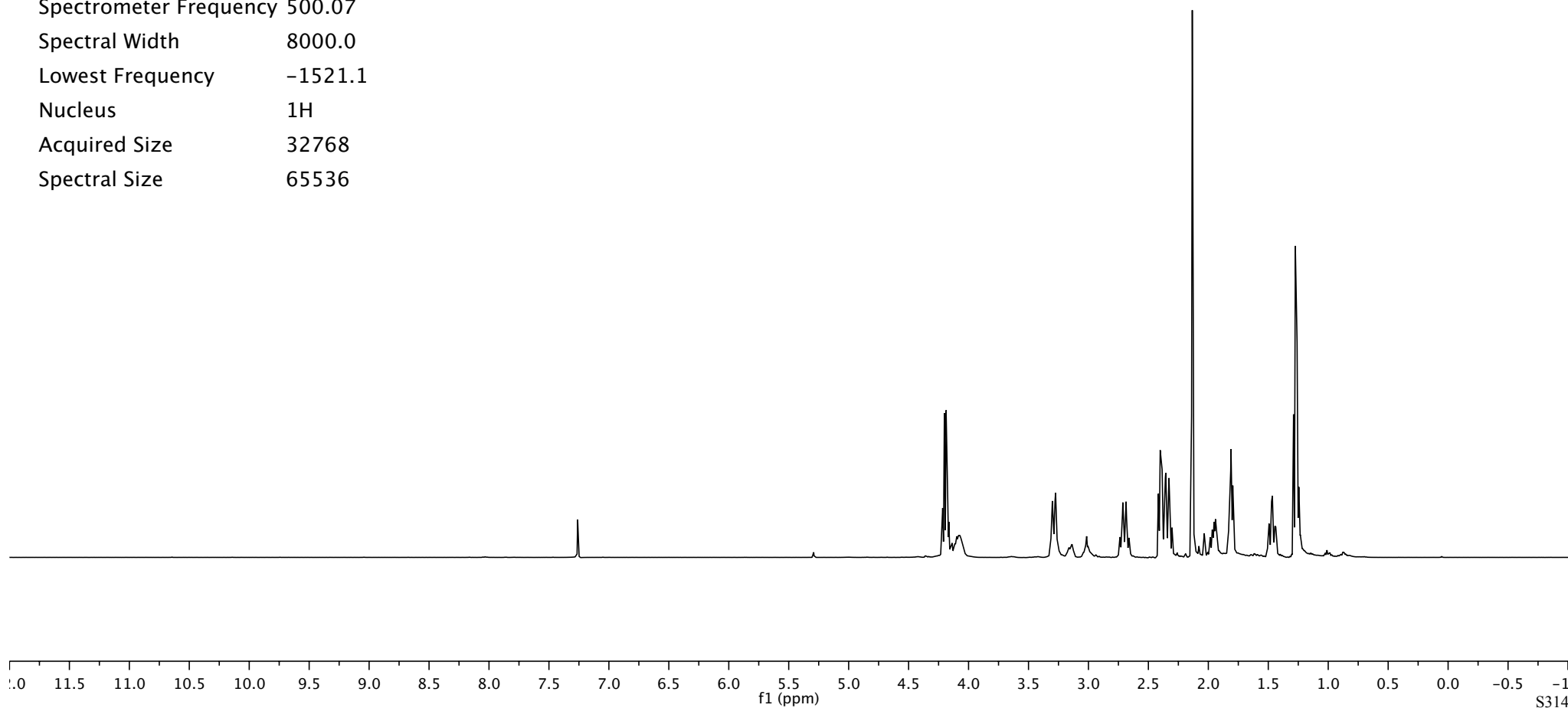
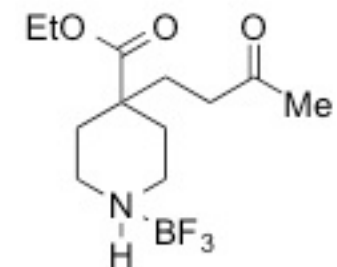


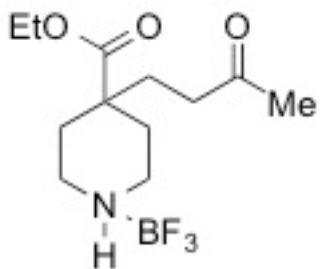


158.68
158.72
158.75
158.79

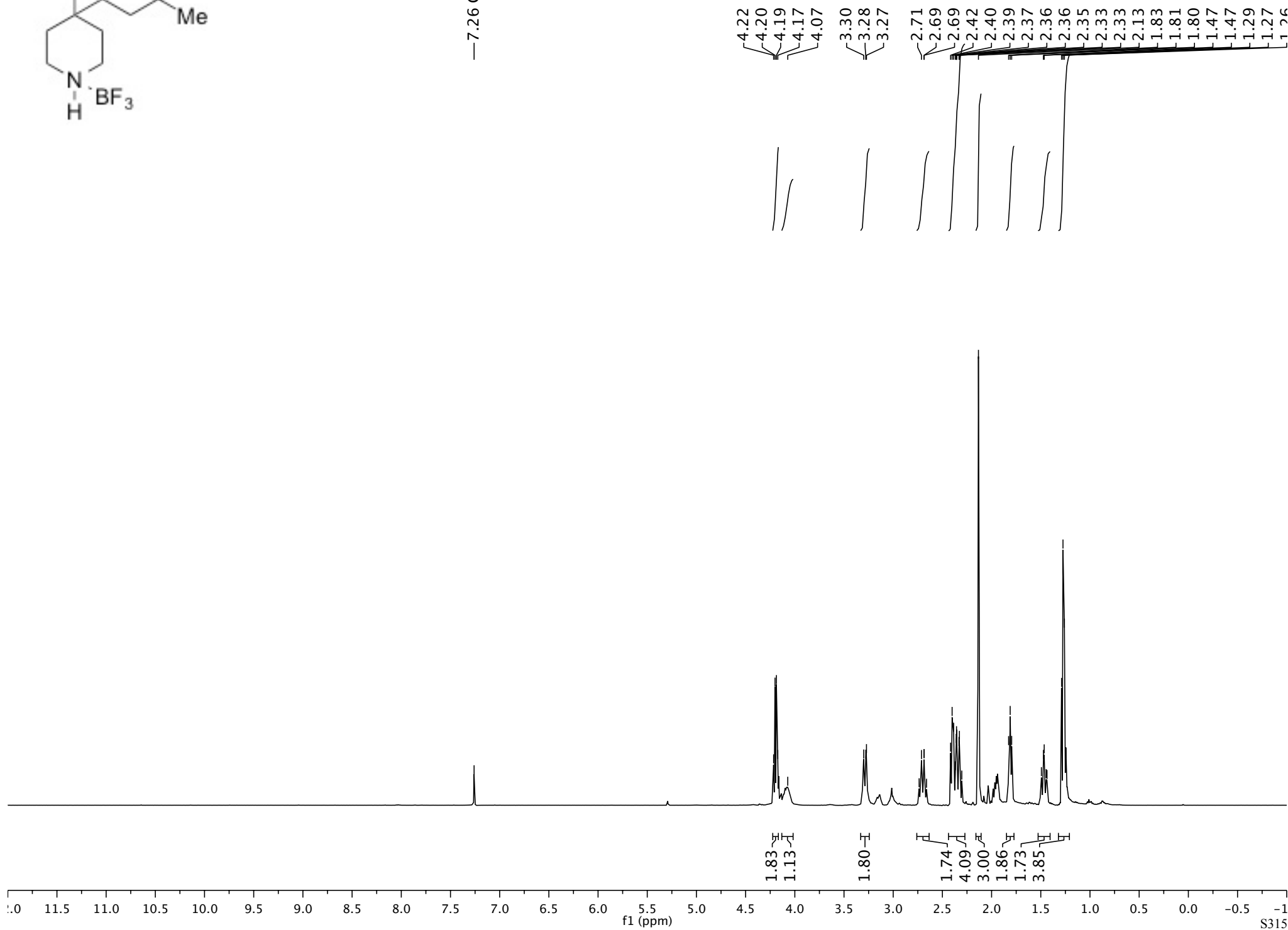


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	26
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	^1H
Acquired Size	32768
Spectral Size	65536

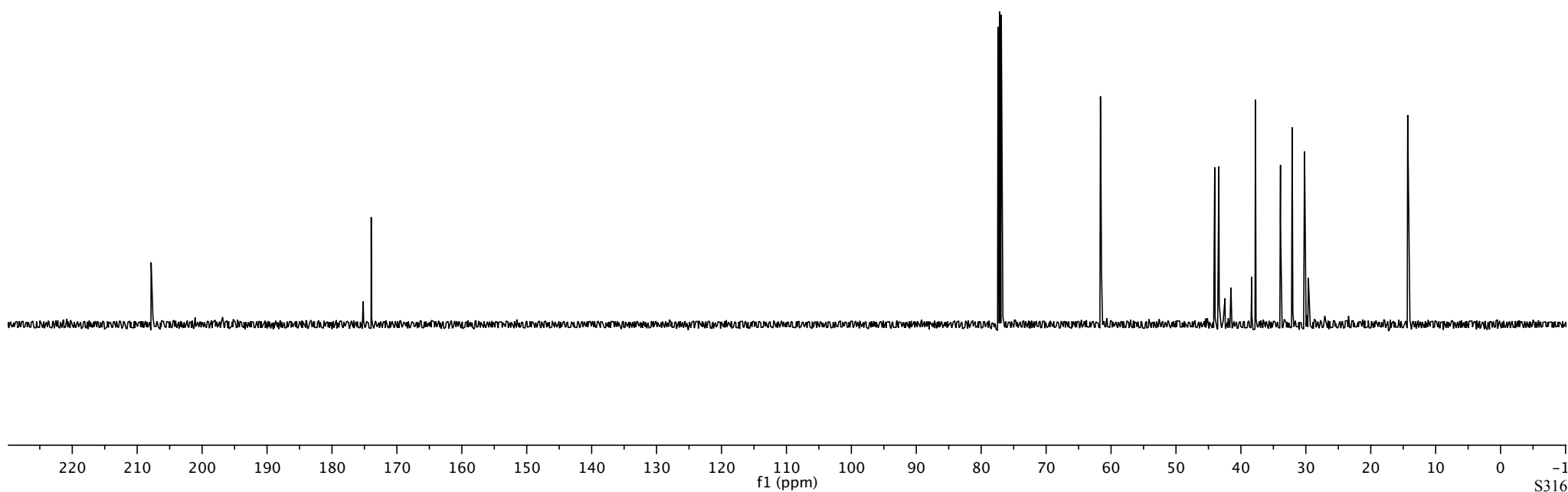
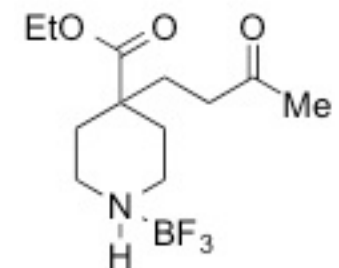


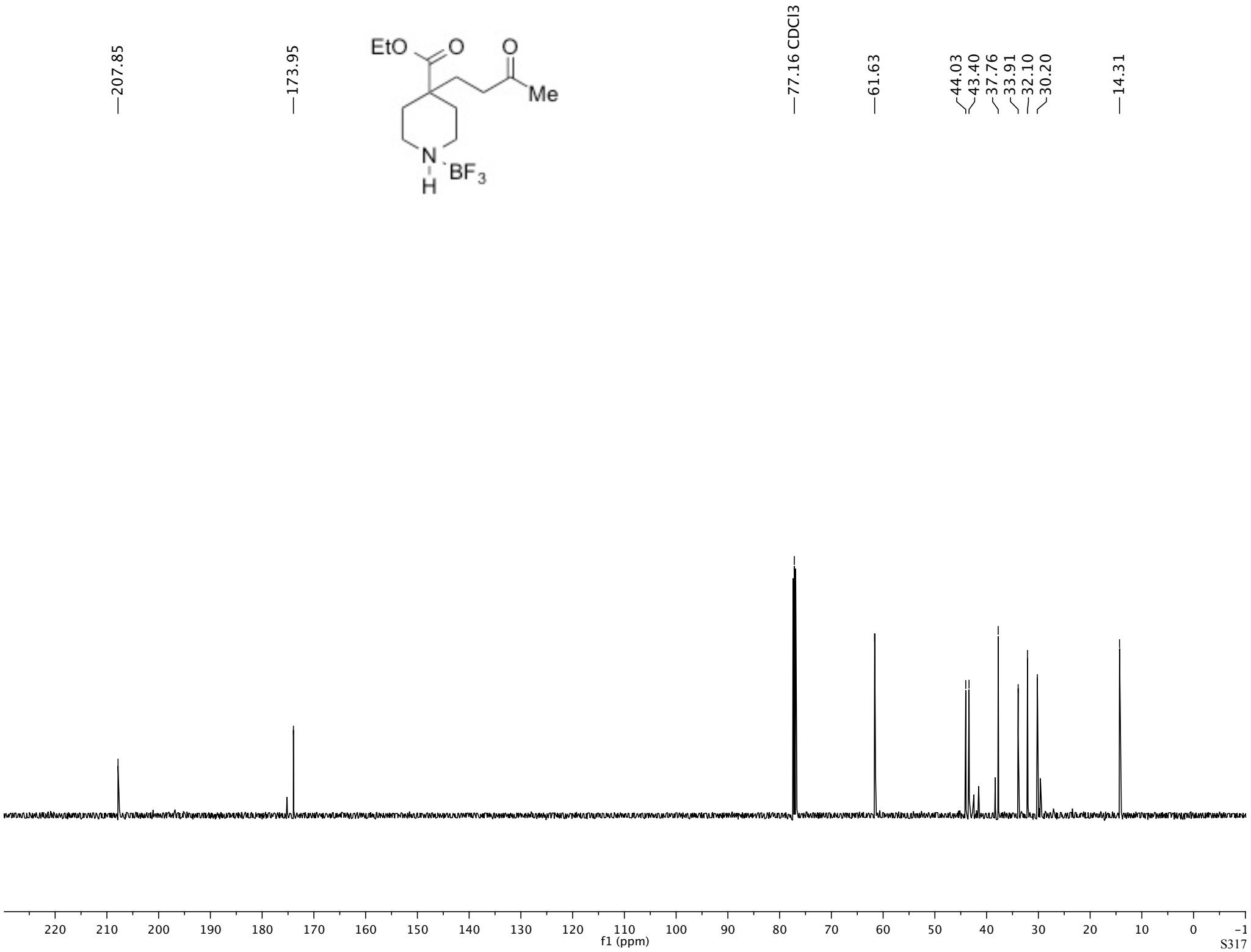


— 7.26 CDCl₃

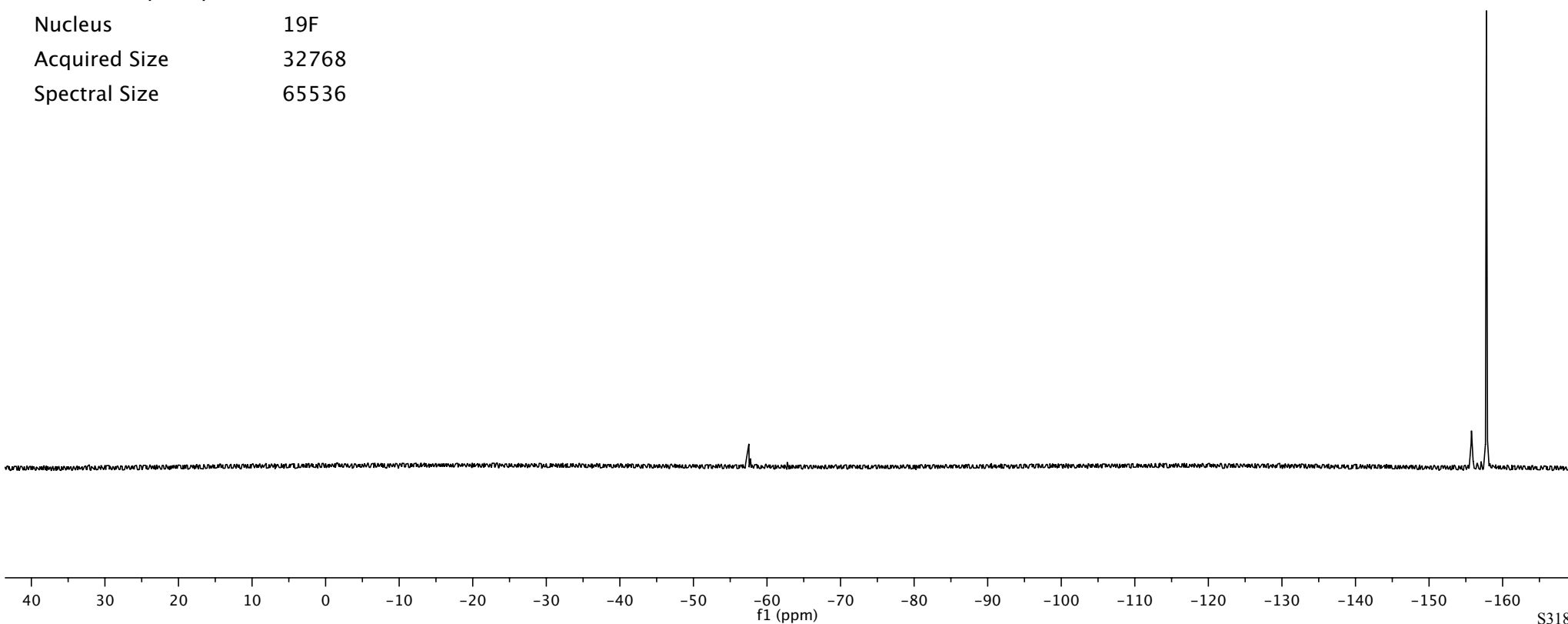
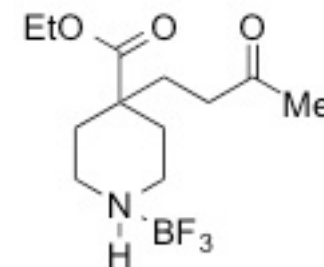


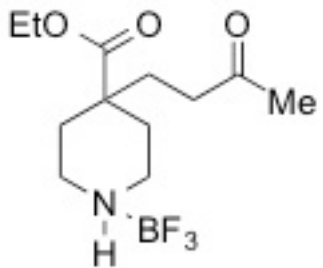
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	520
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1275.1
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



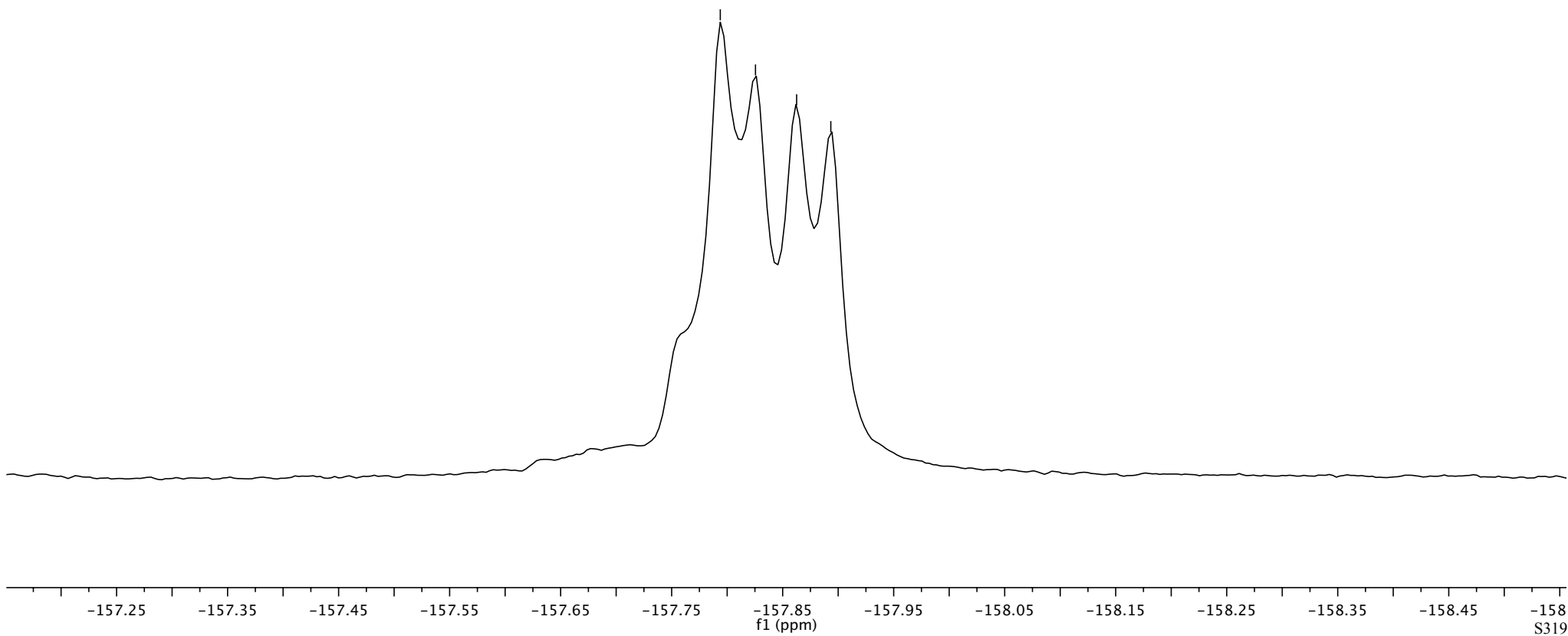


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	132
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency	-79501.3
Nucleus	¹⁹ F
Acquired Size	32768
Spectral Size	65536

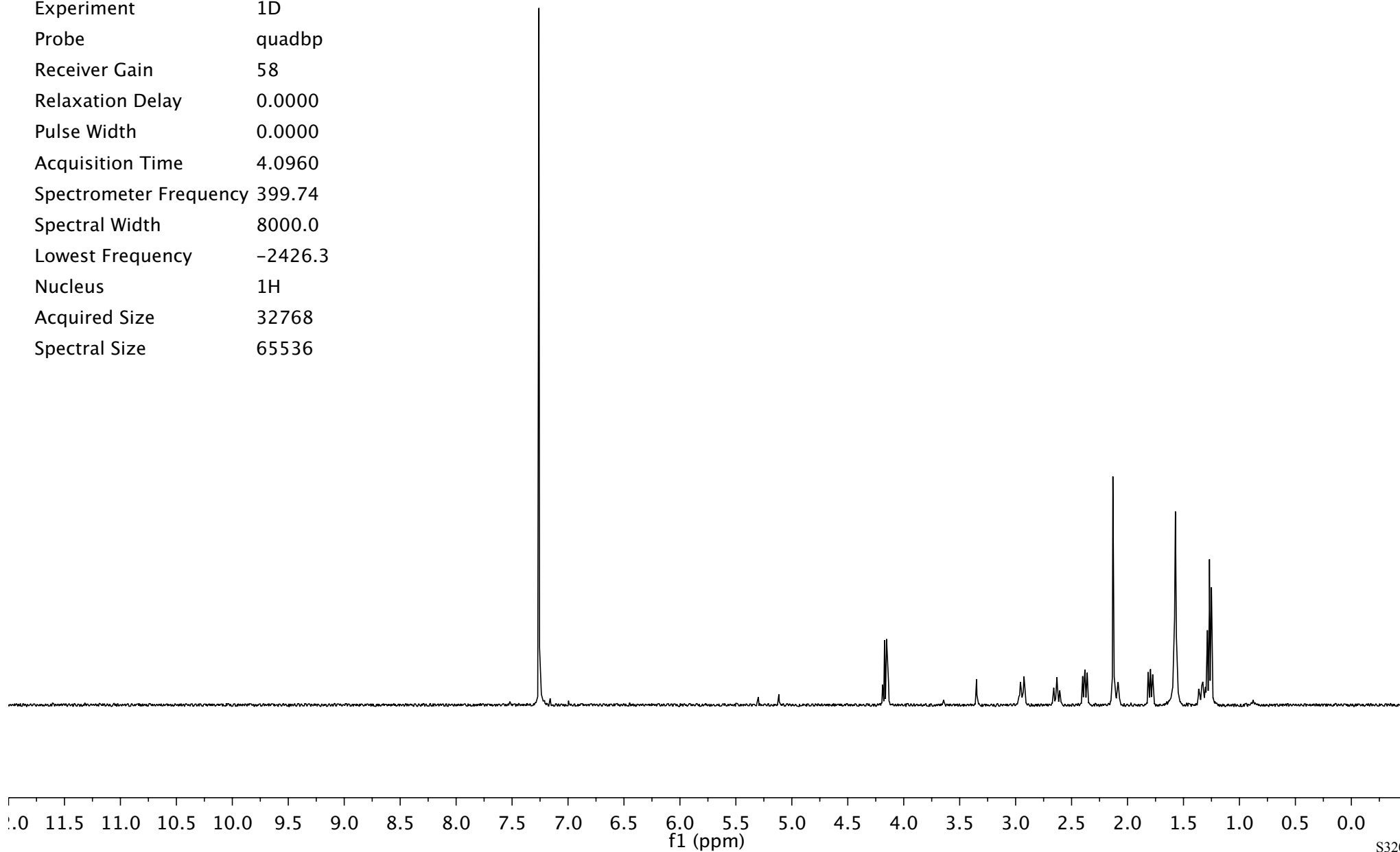
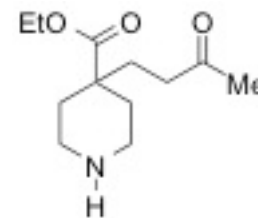


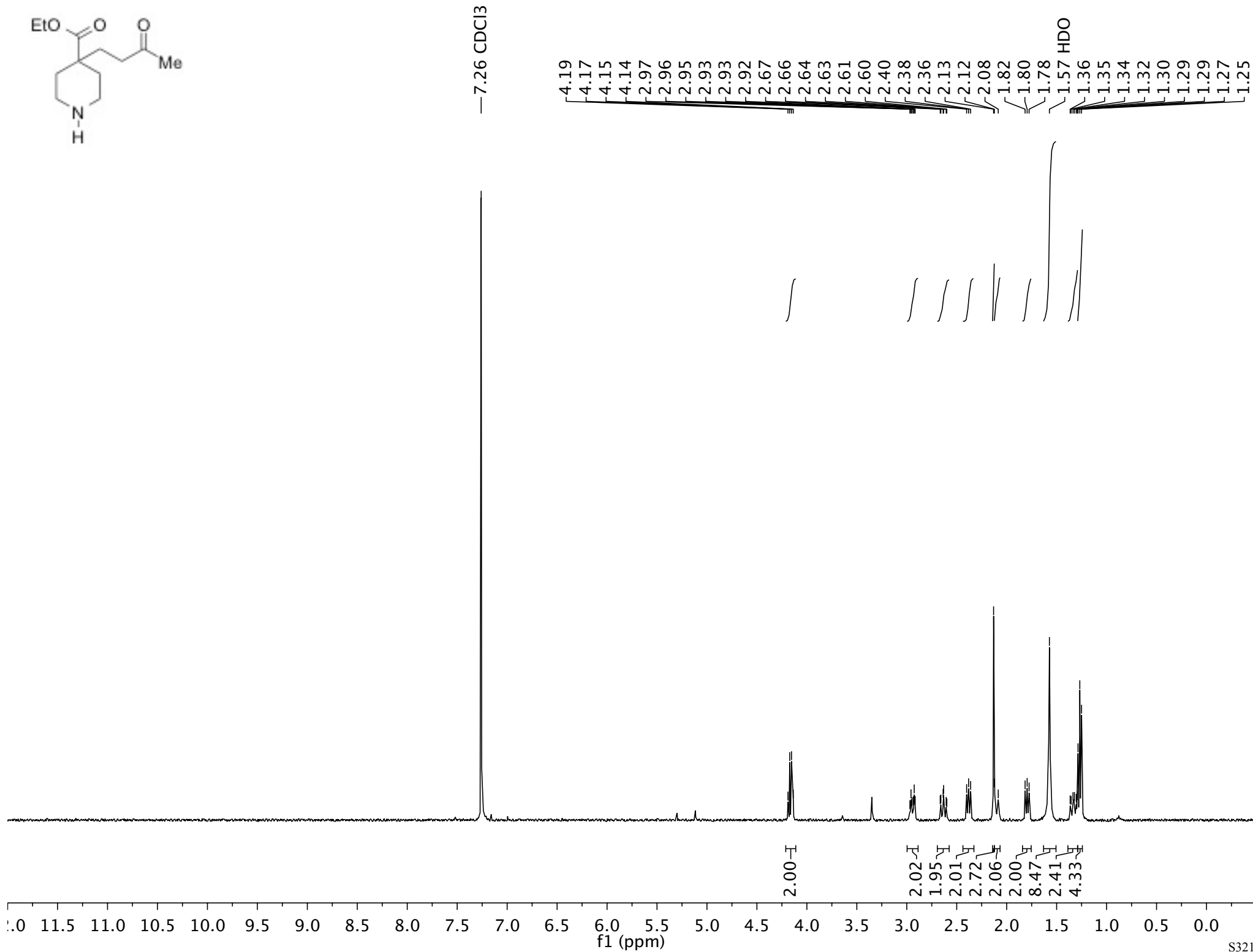
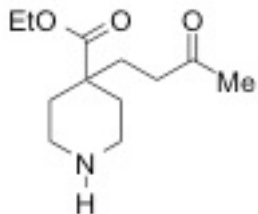


157.79
157.83
157.86
157.89

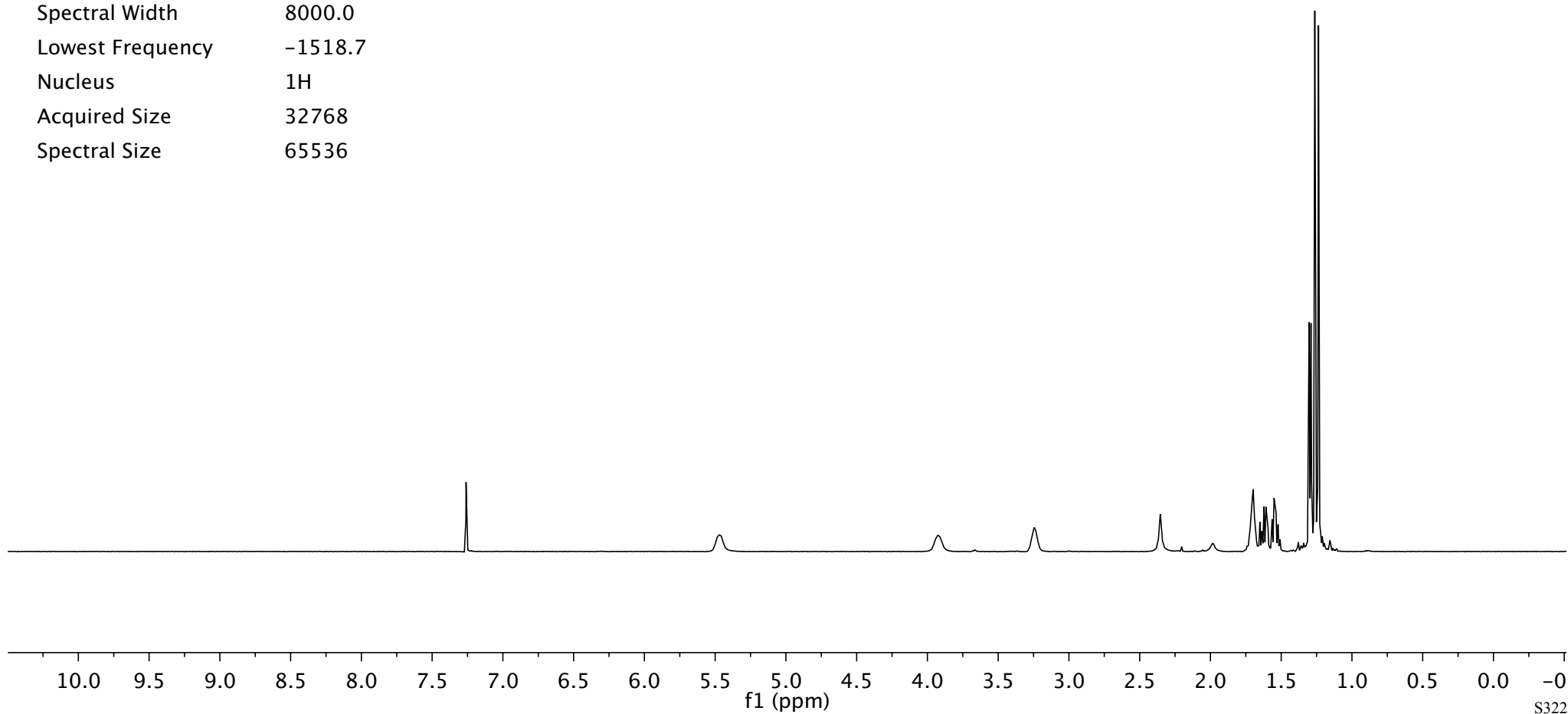
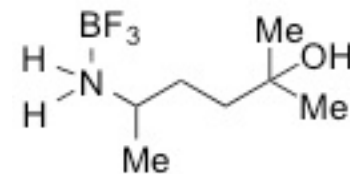


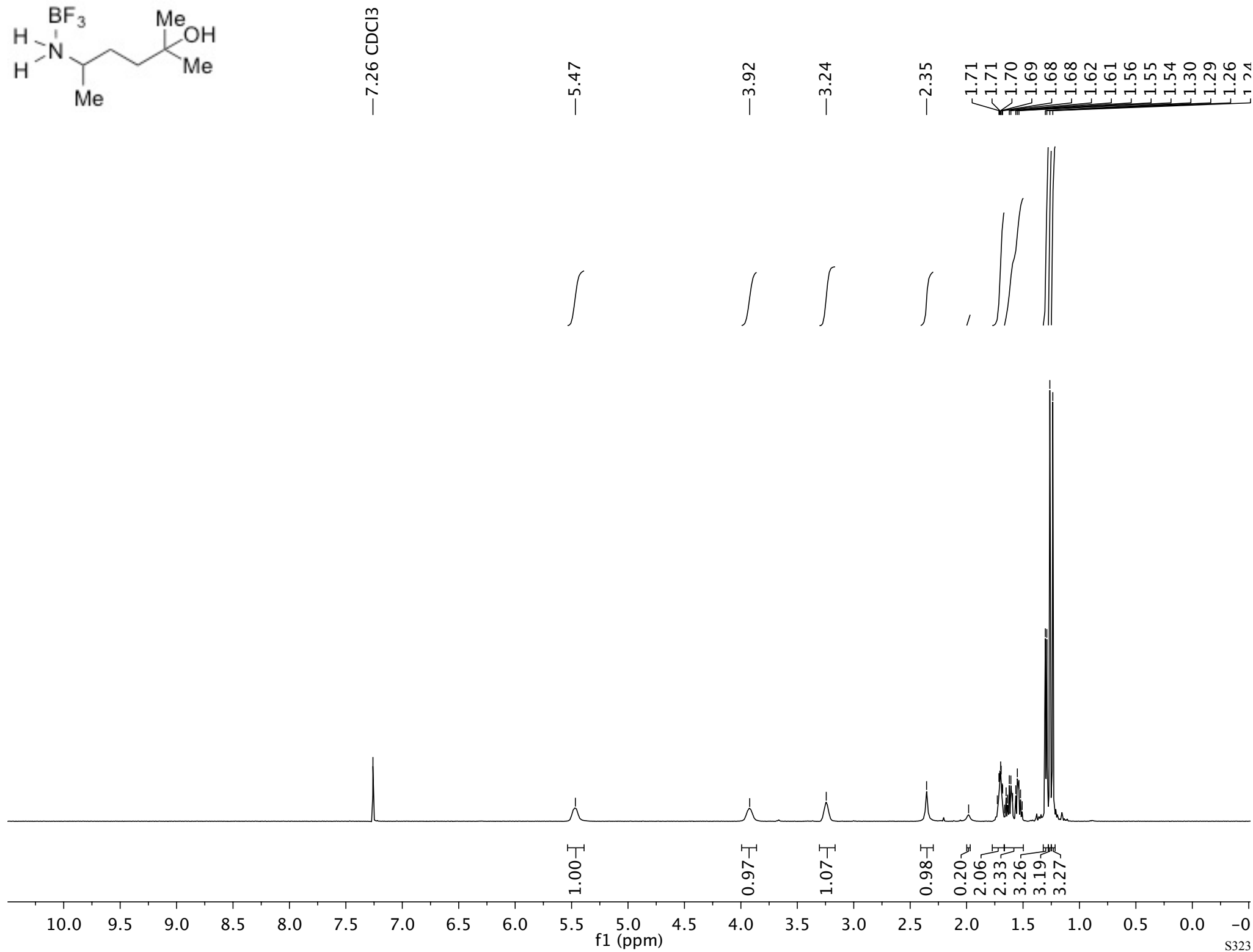
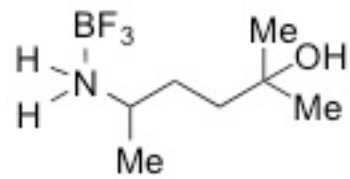
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quadbp
Receiver Gain	58
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	399.74
Spectral Width	8000.0
Lowest Frequency	-2426.3
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



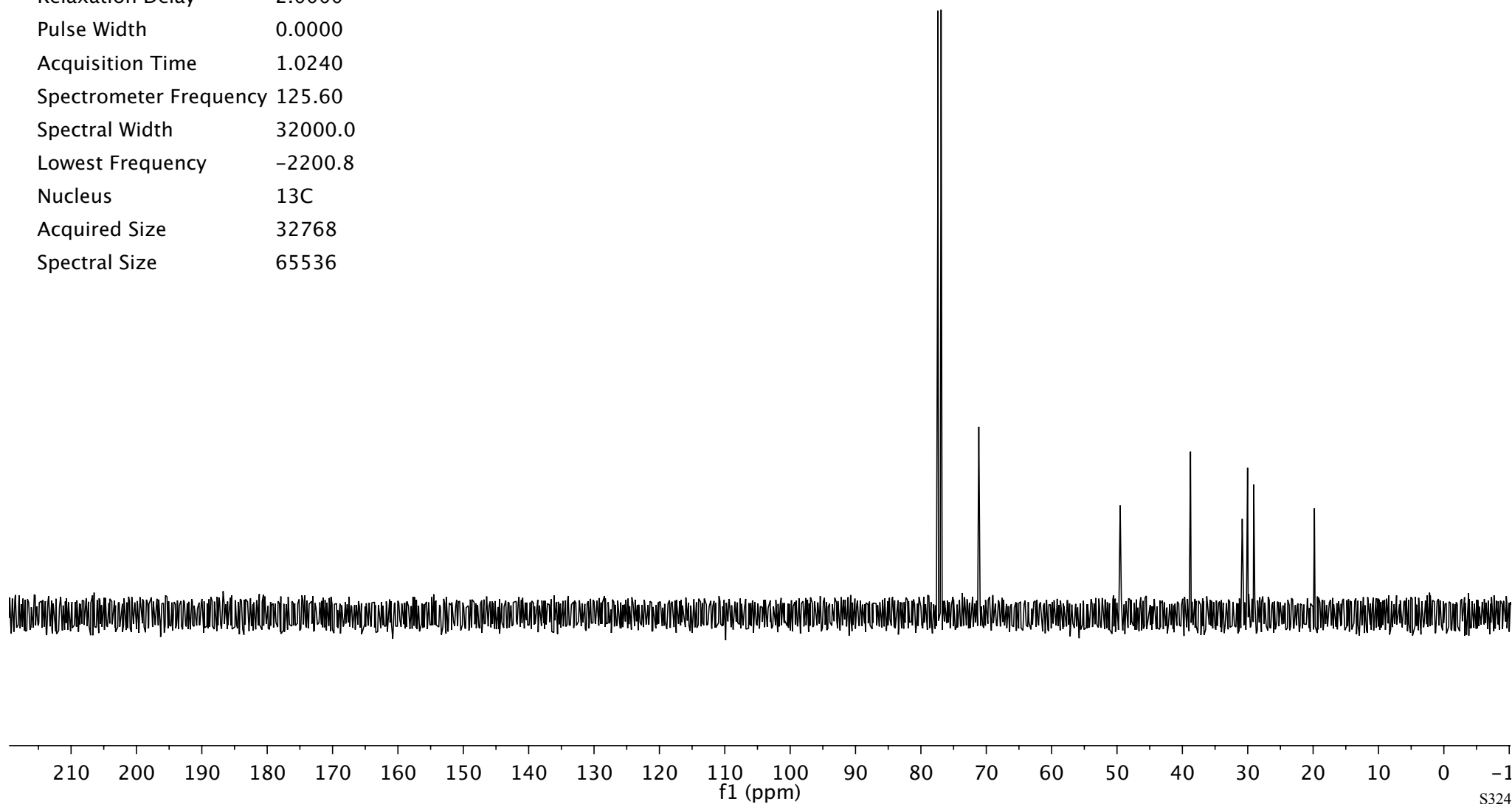
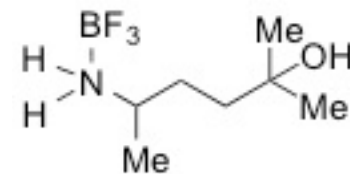


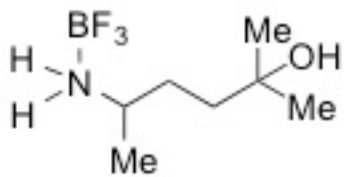
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	56
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	499.43
Spectral Width	8000.0
Lowest Frequency	-1518.7
Nucleus	1H
Acquired Size	32768
Spectral Size	65536





Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2200.8
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536





77.41 CDCl₃
77.16 CDCl₃
76.91 CDCl₃
71.14

49.51

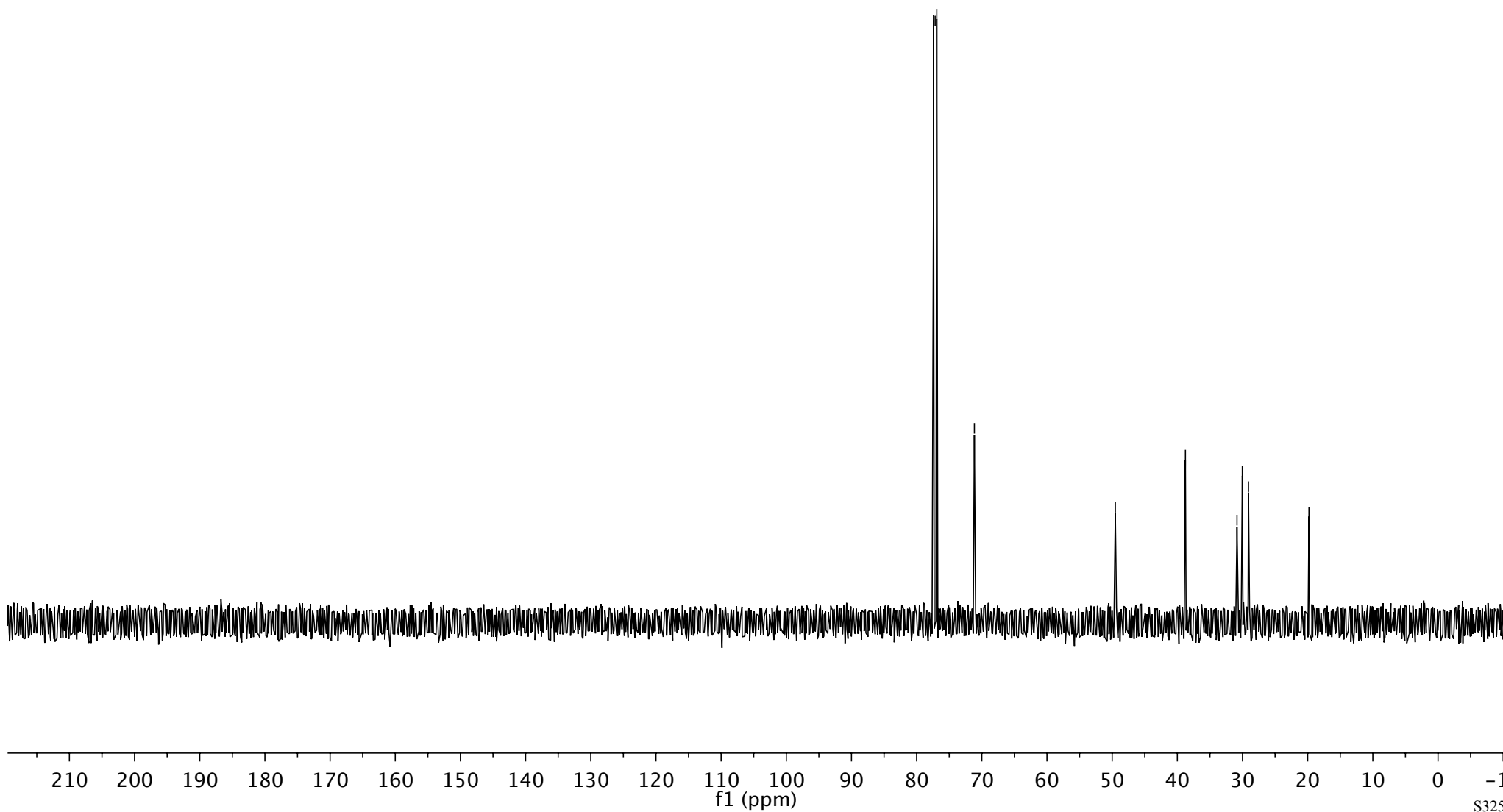
38.76

30.84

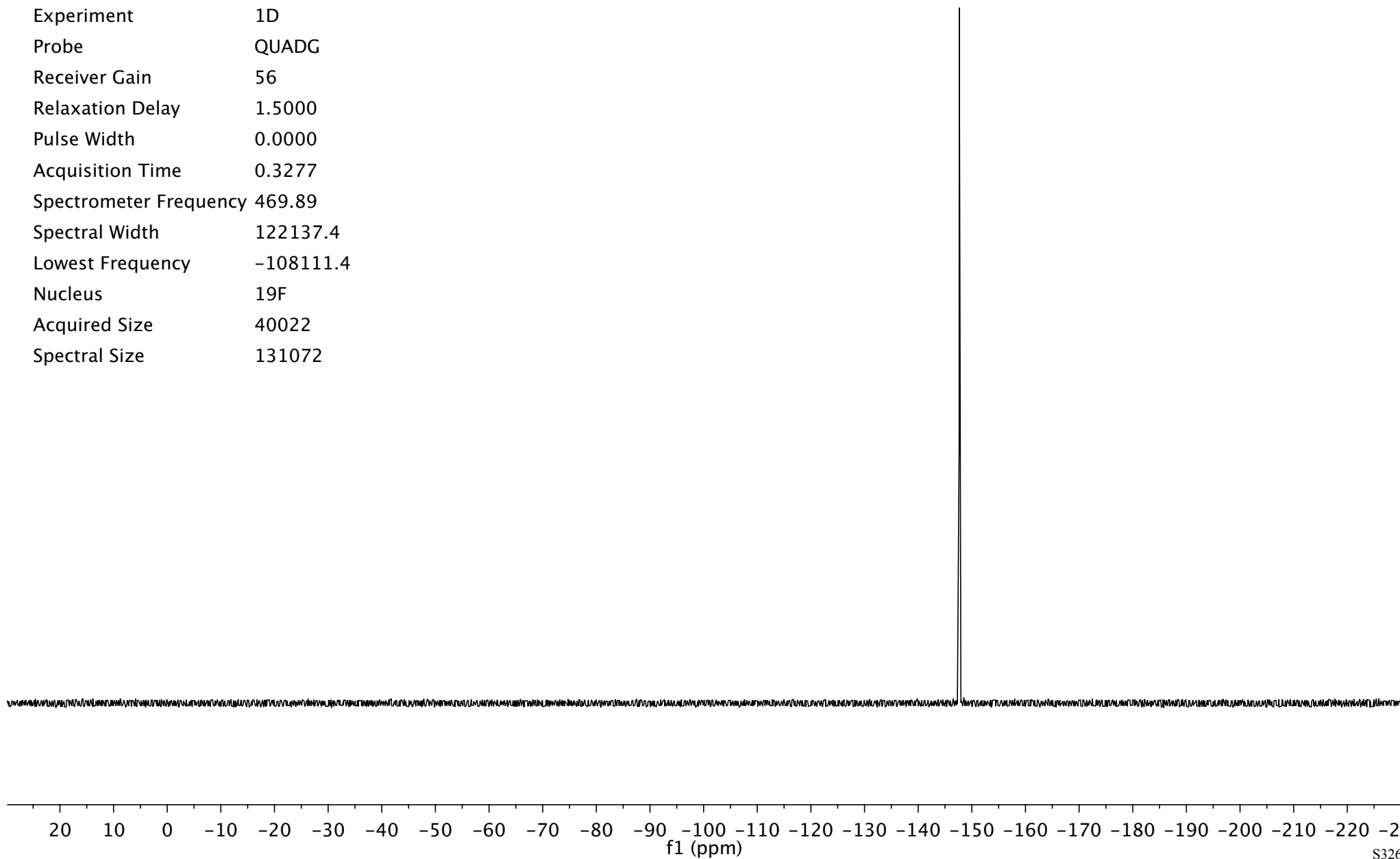
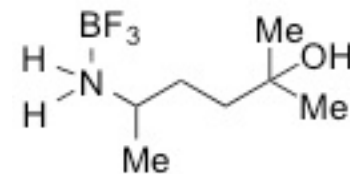
30.03

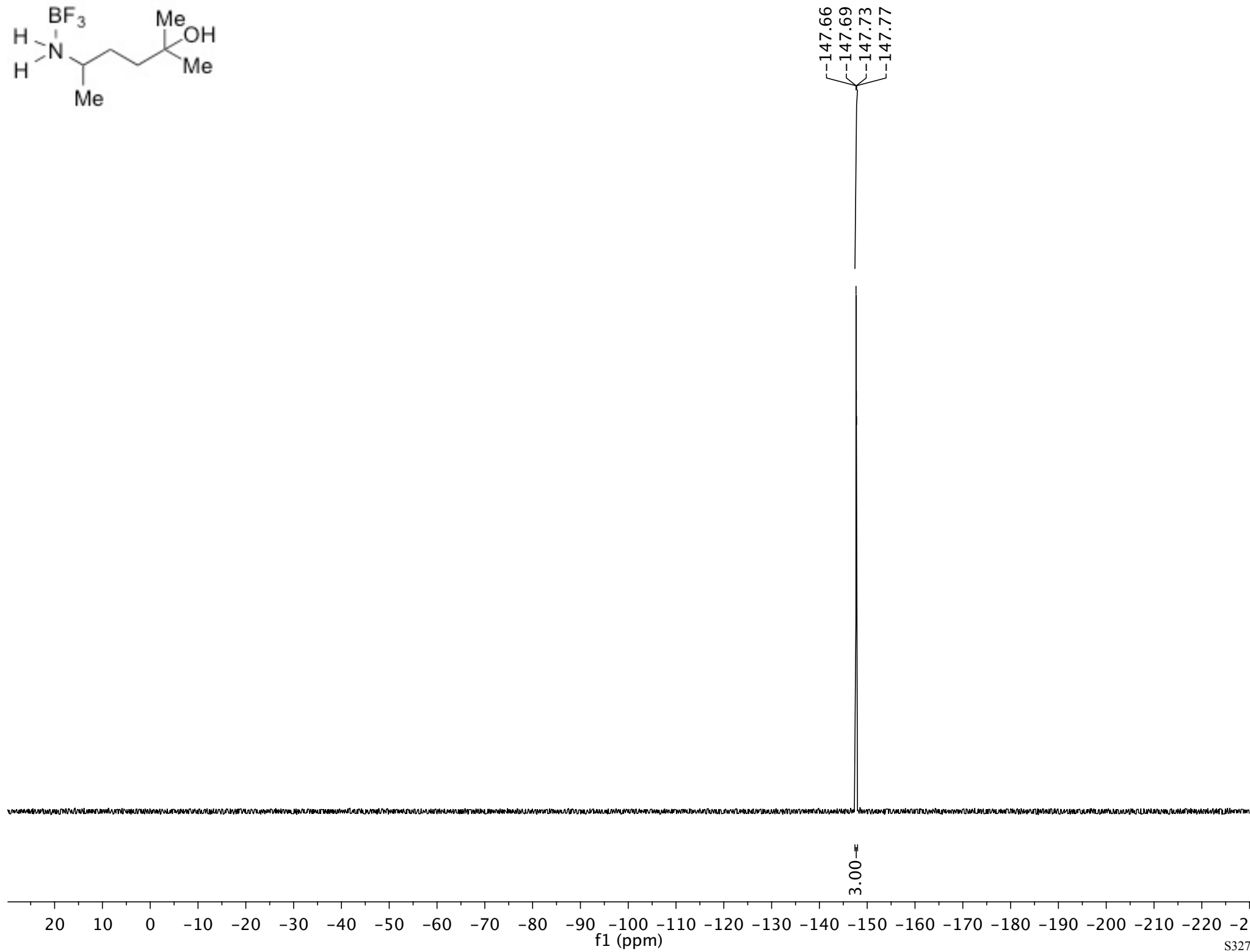
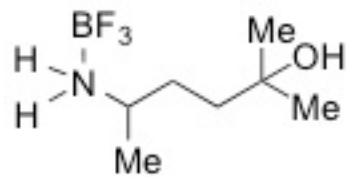
29.08

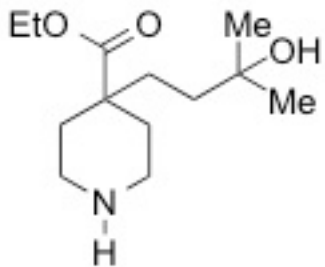
19.80



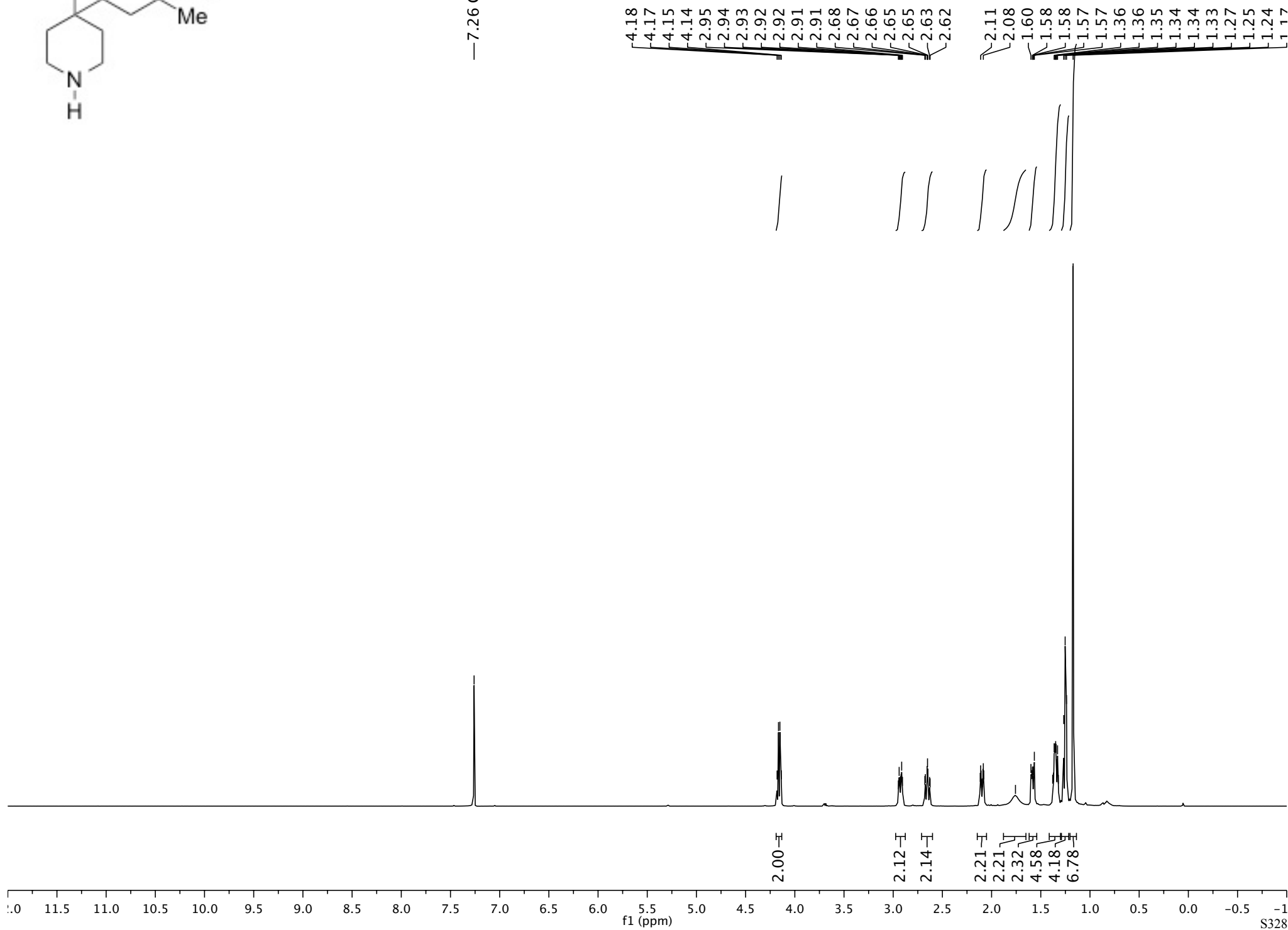
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	56
Relaxation Delay	1.5000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	469.89
Spectral Width	122137.4
Lowest Frequency	-108111.4
Nucleus	19F
Acquired Size	40022
Spectral Size	131072



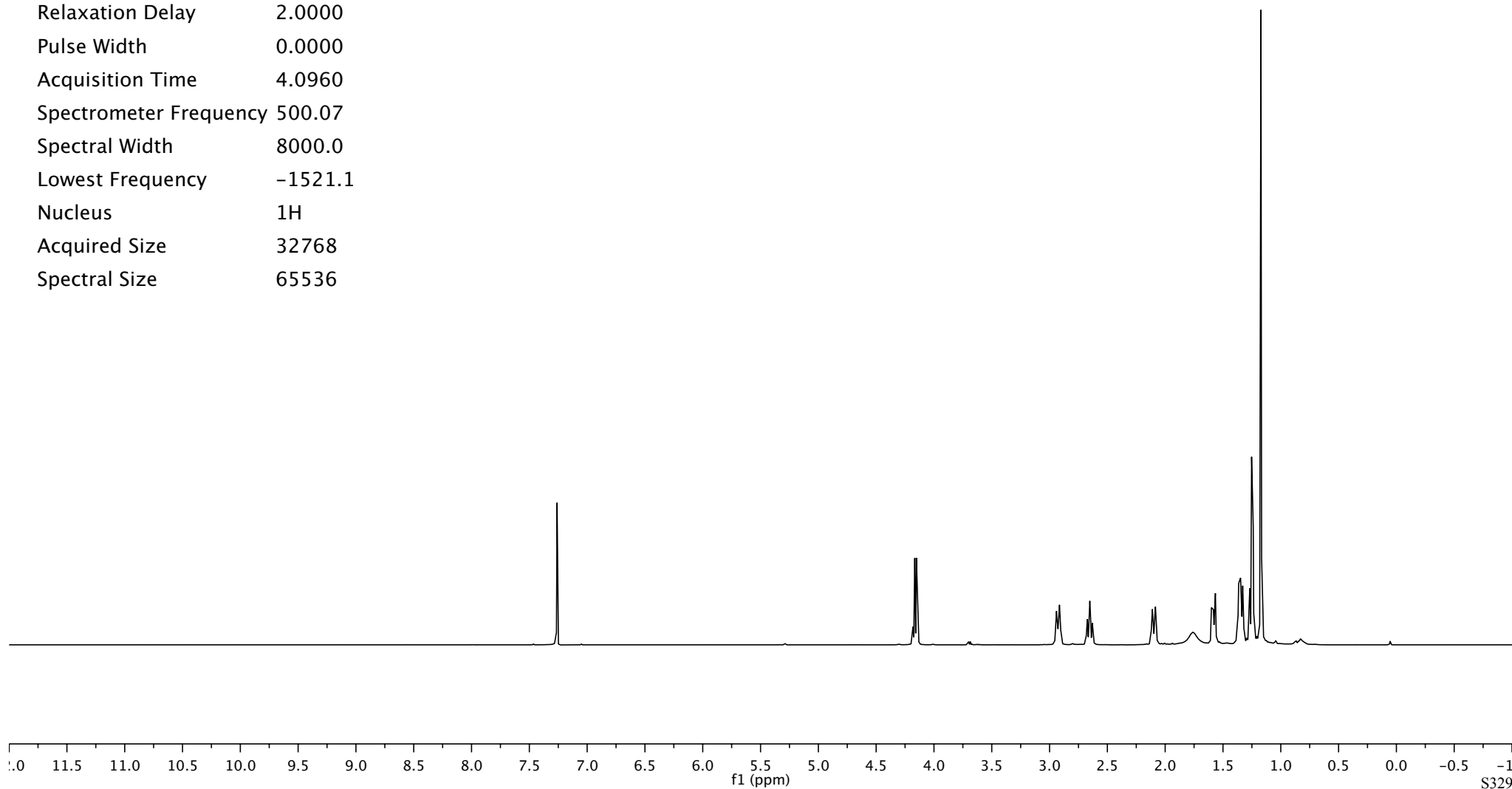
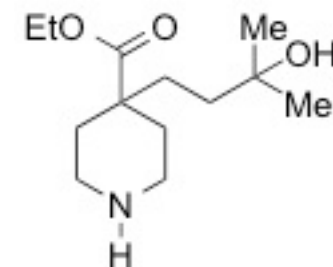




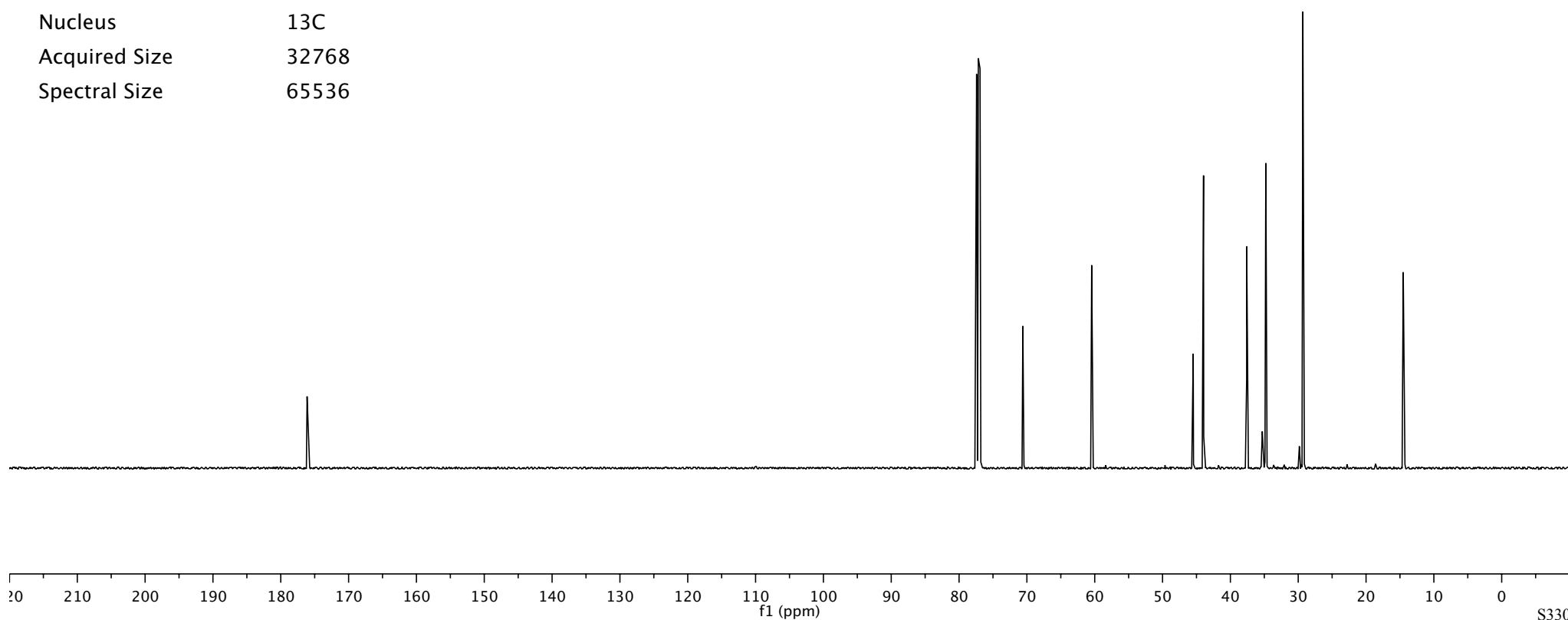
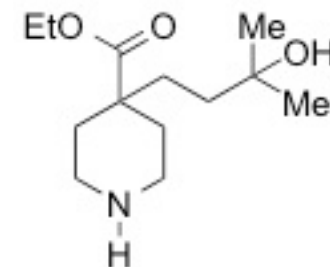
— 7.26 CDCl₃

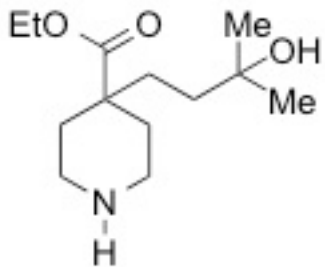


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	28
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	11999
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1273.8
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536





—176.12

—77.16 CDCl₃

—70.59

—60.45

—45.48

—43.96

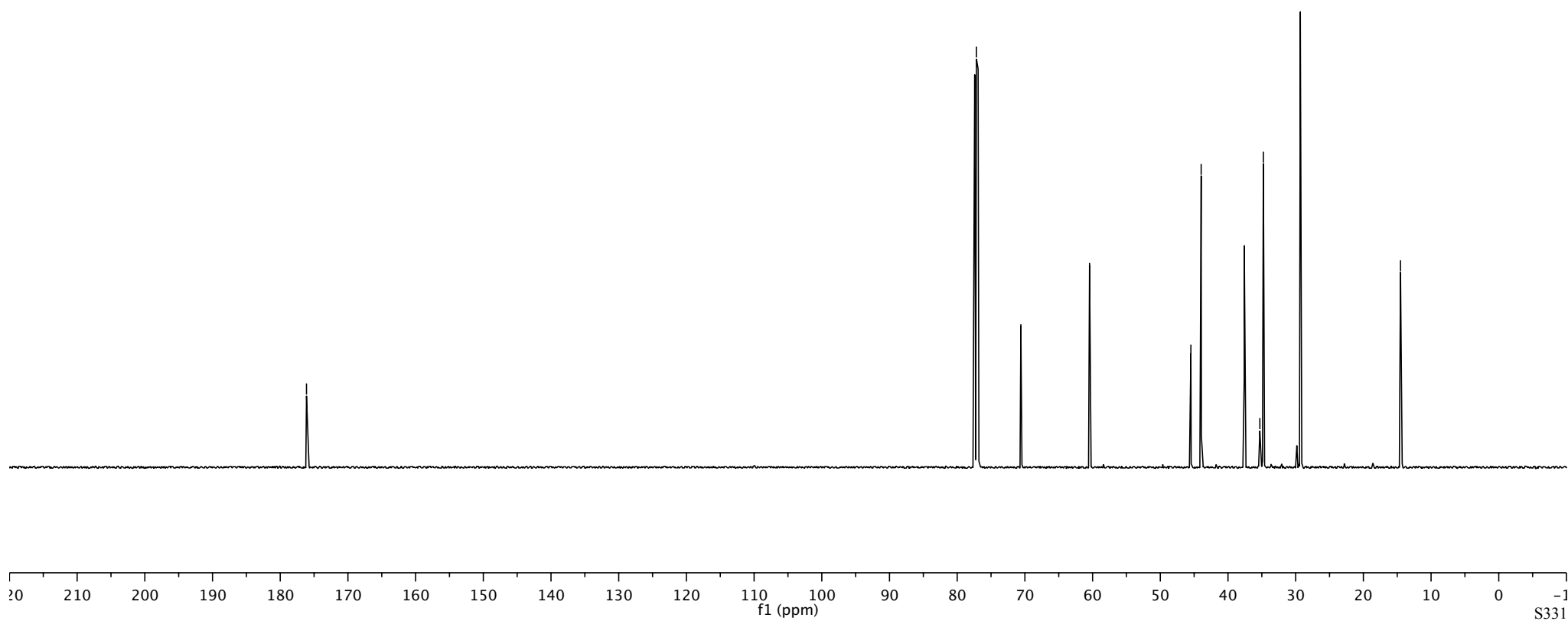
—37.59

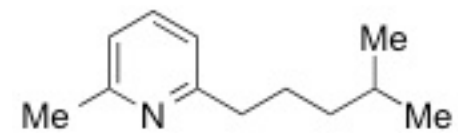
—35.29

—34.78

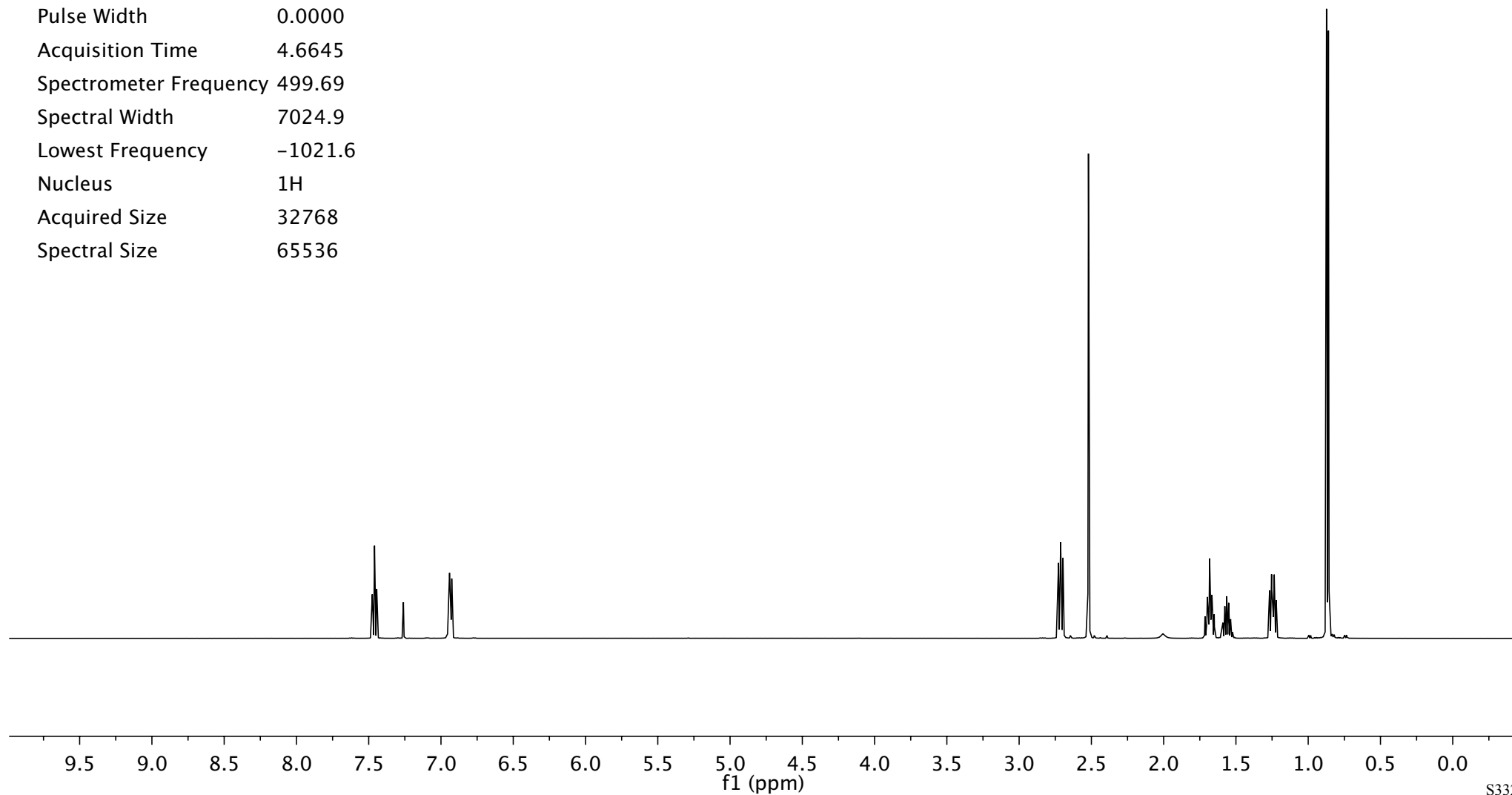
—29.31

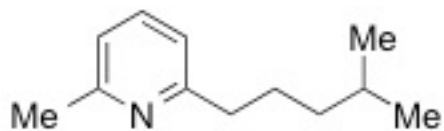
—14.52





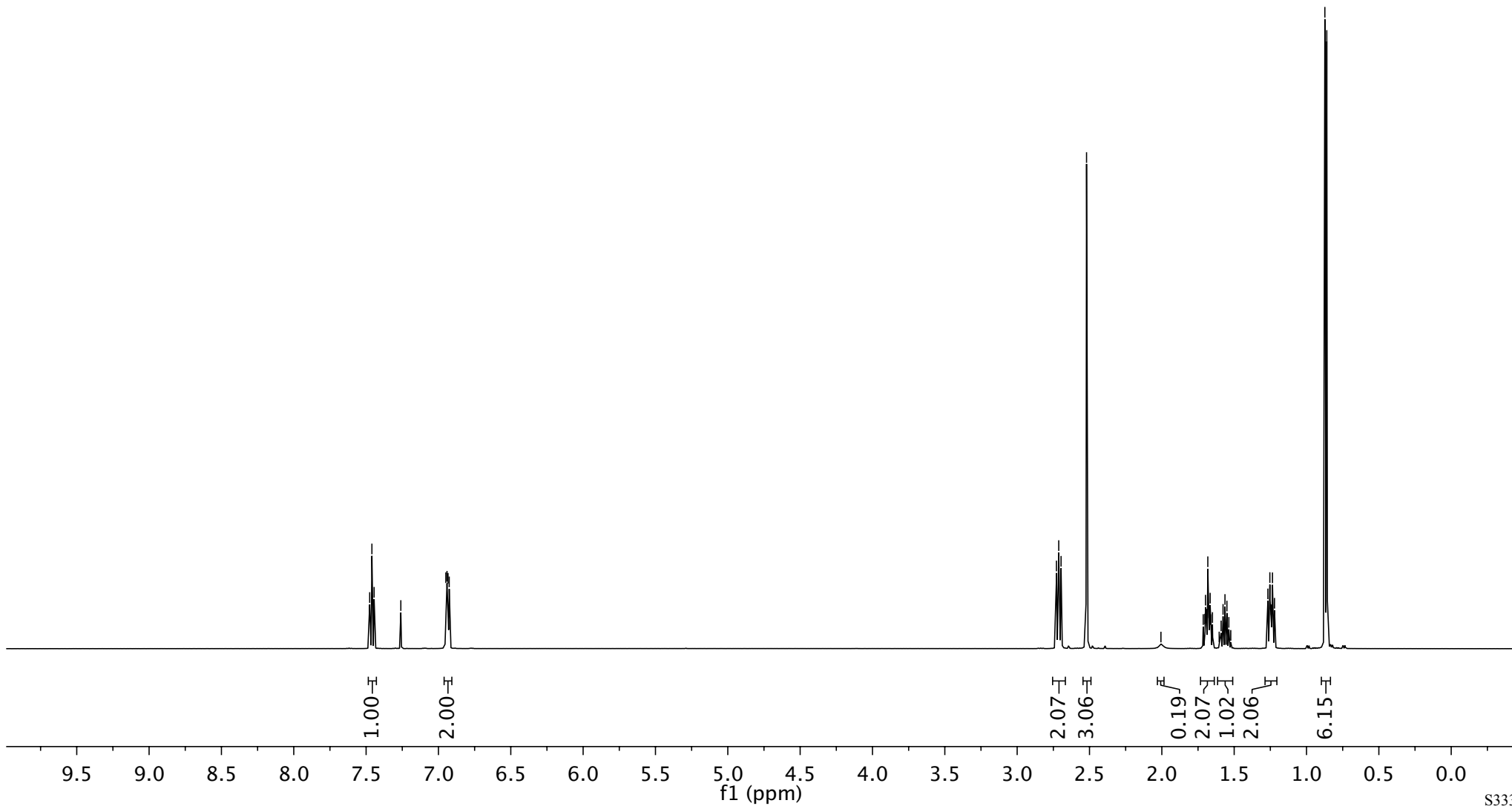
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	42
Relaxation Delay	5.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.69
Spectral Width	7024.9
Lowest Frequency	-1021.6
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



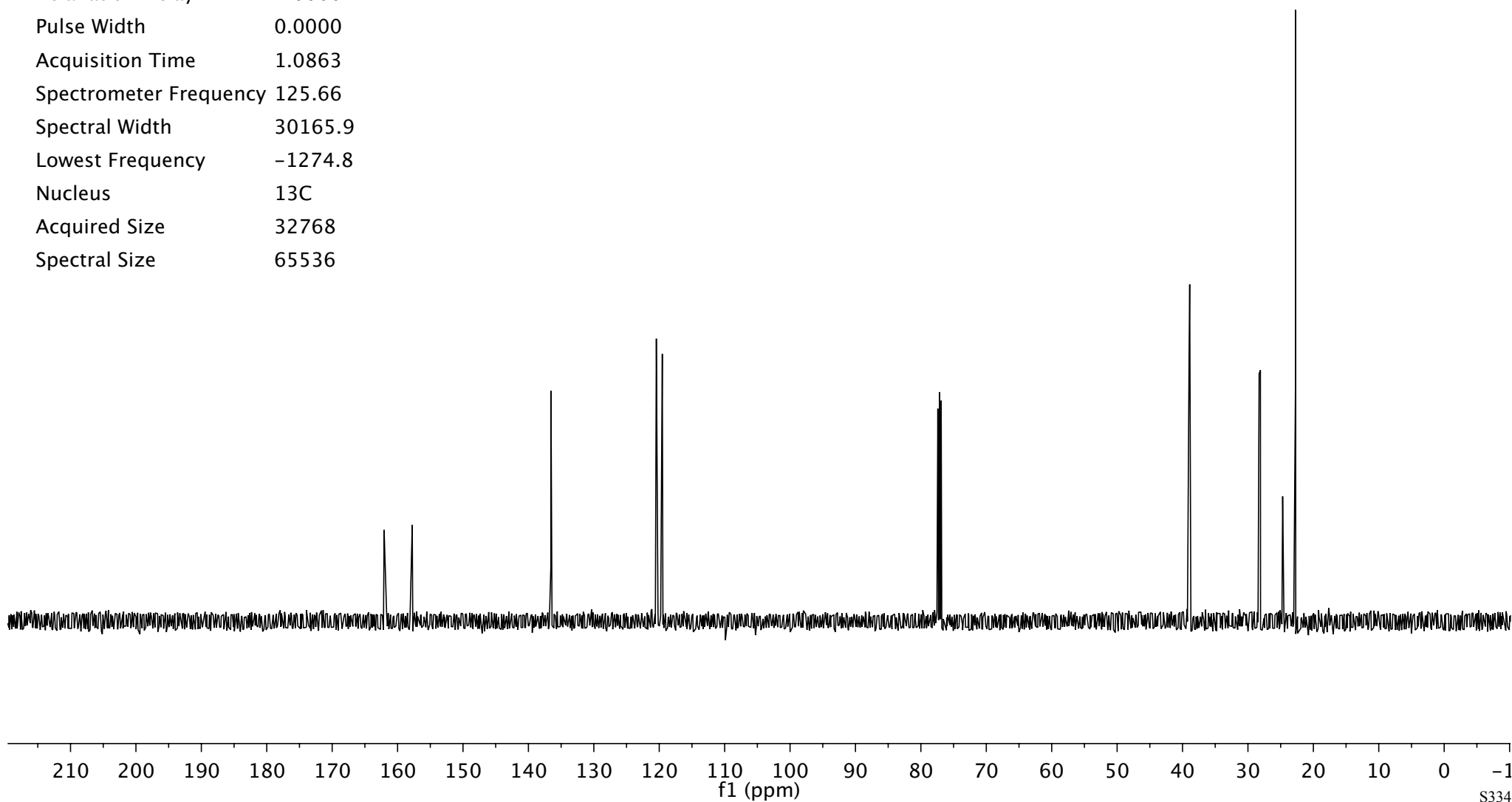
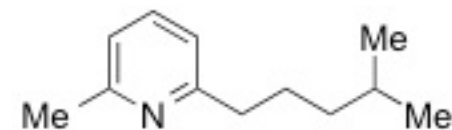


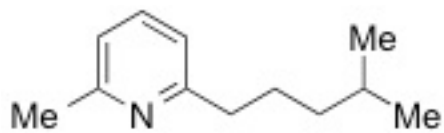
7.48
7.46
7.44
7.26 CDCl₃
6.95
6.94
6.93
6.93

2.73
2.71
2.70
2.52
2.01
1.71
1.70
1.70
1.69
1.68
1.67
1.67
1.67
1.66
1.65
1.60
1.59
1.58
1.56
1.55
1.54
1.52
1.27
1.25
1.24
1.24
1.22
0.87
0.86



Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1274.8
Nucleus	13C
Acquired Size	32768
Spectral Size	65536





—162.07
—157.77

—136.56

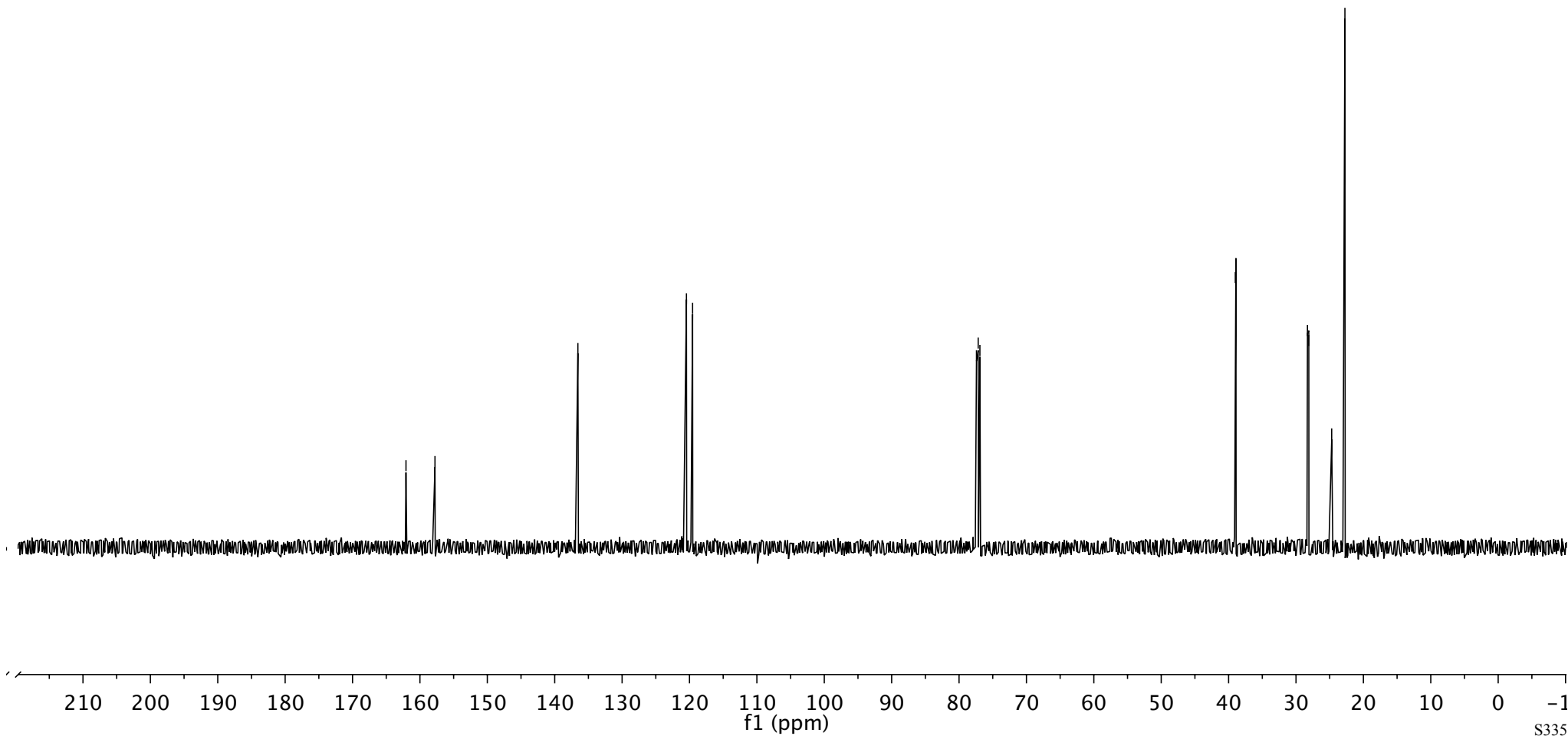
—120.45
—119.54

77.41 CDCl₃
77.16 CDCl₃
76.91 CDCl₃

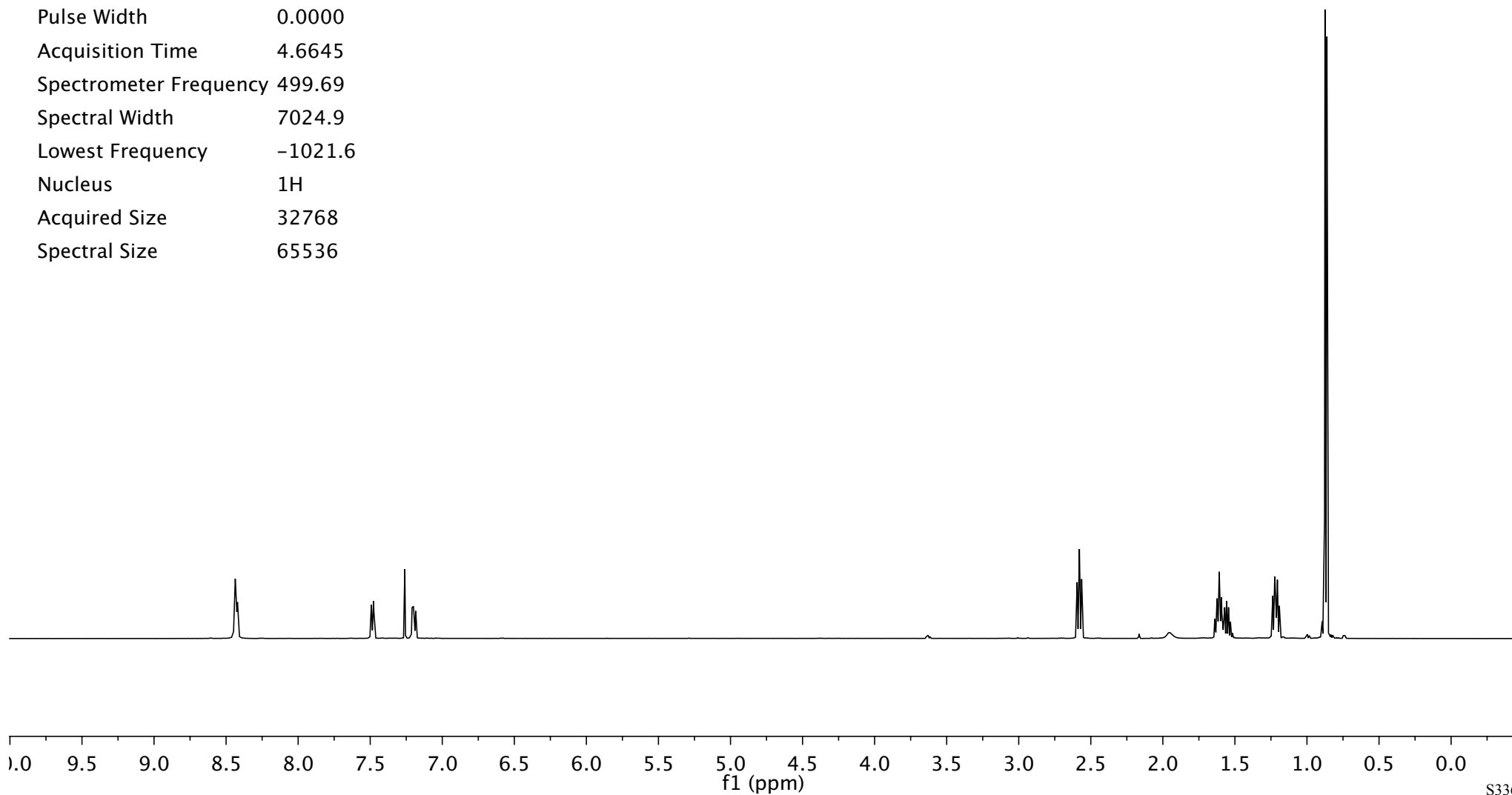
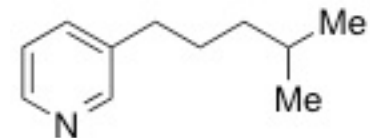
39.01
38.92

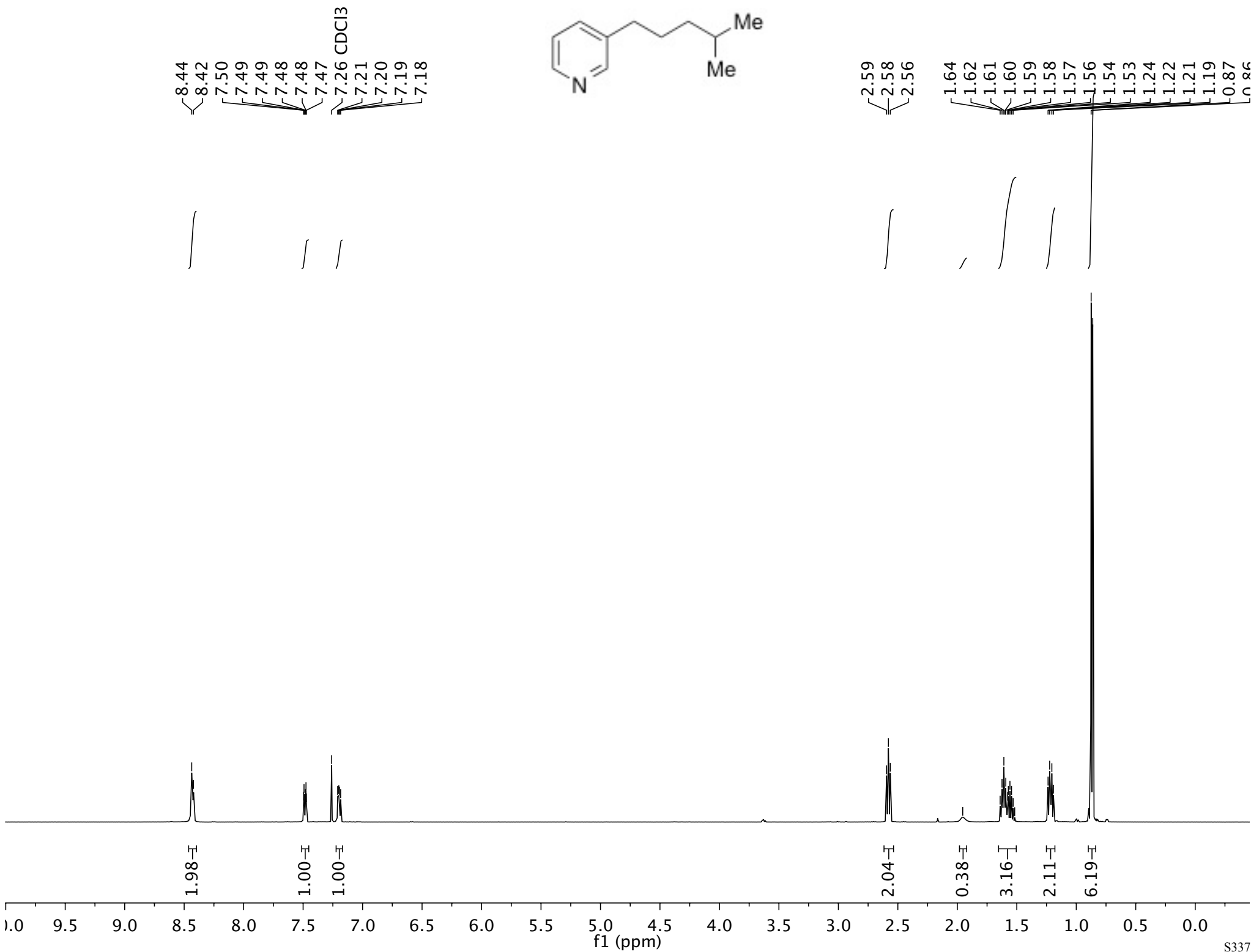
28.30
28.10

24.70
22.74

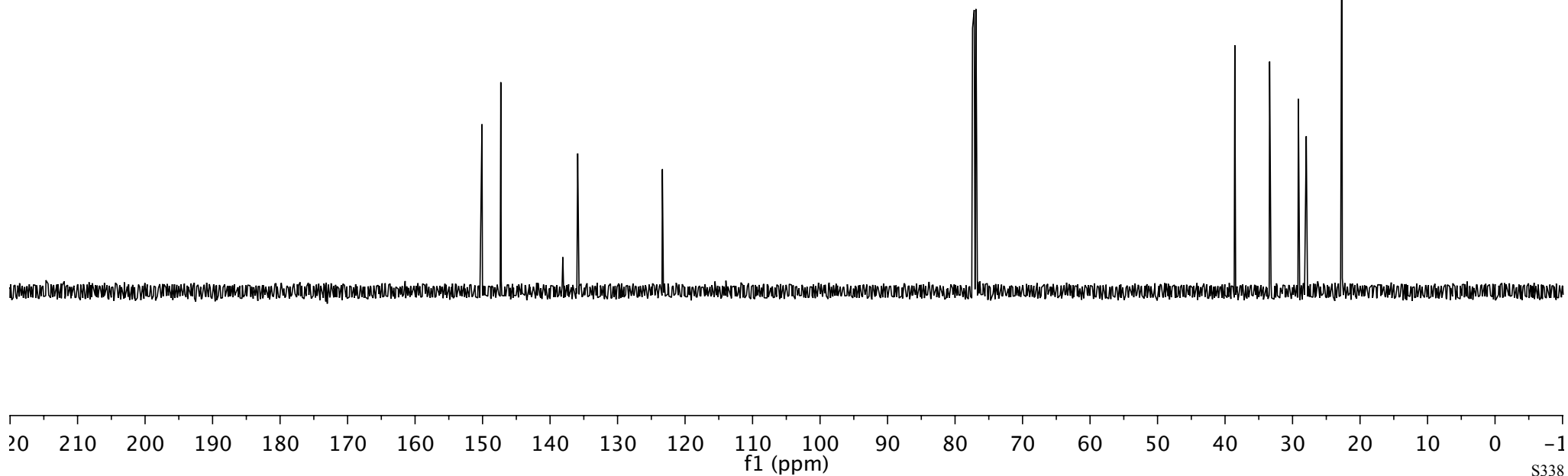
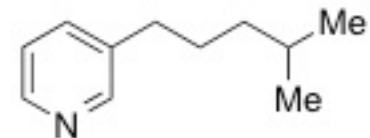


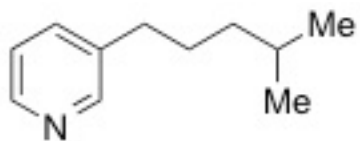
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	46
Relaxation Delay	5.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.69
Spectral Width	7024.9
Lowest Frequency	-1021.6
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



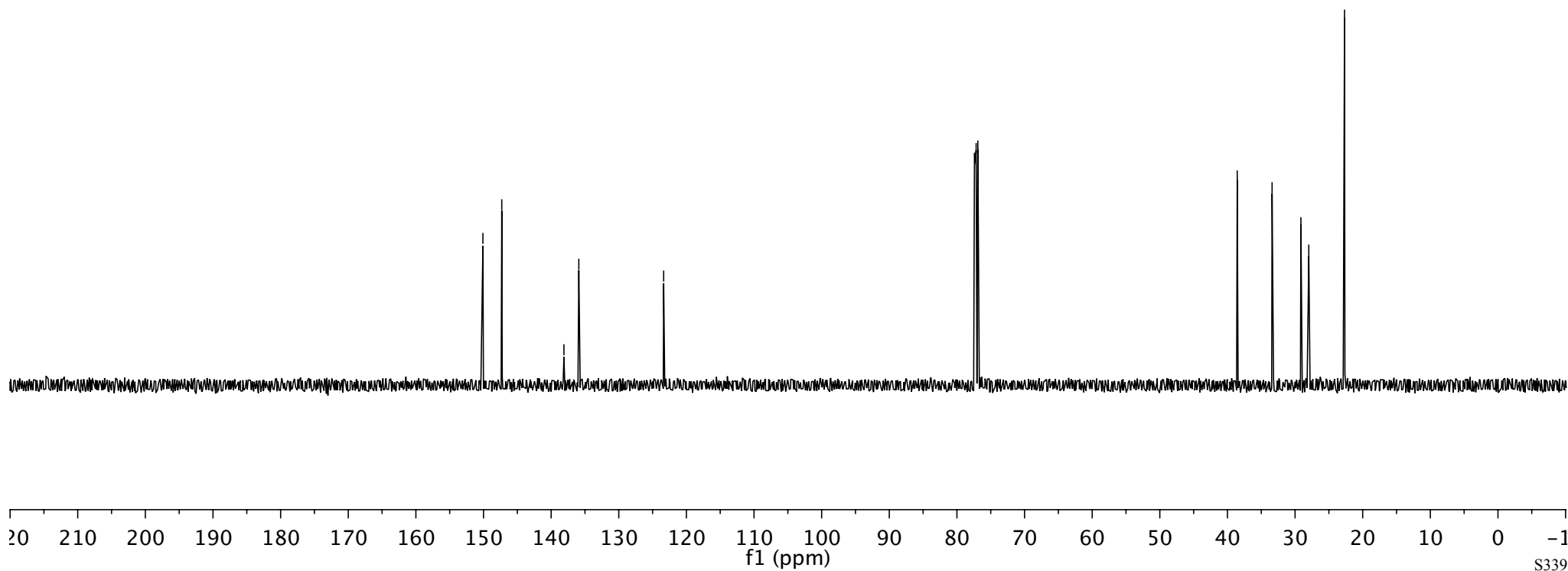


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1273.3
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

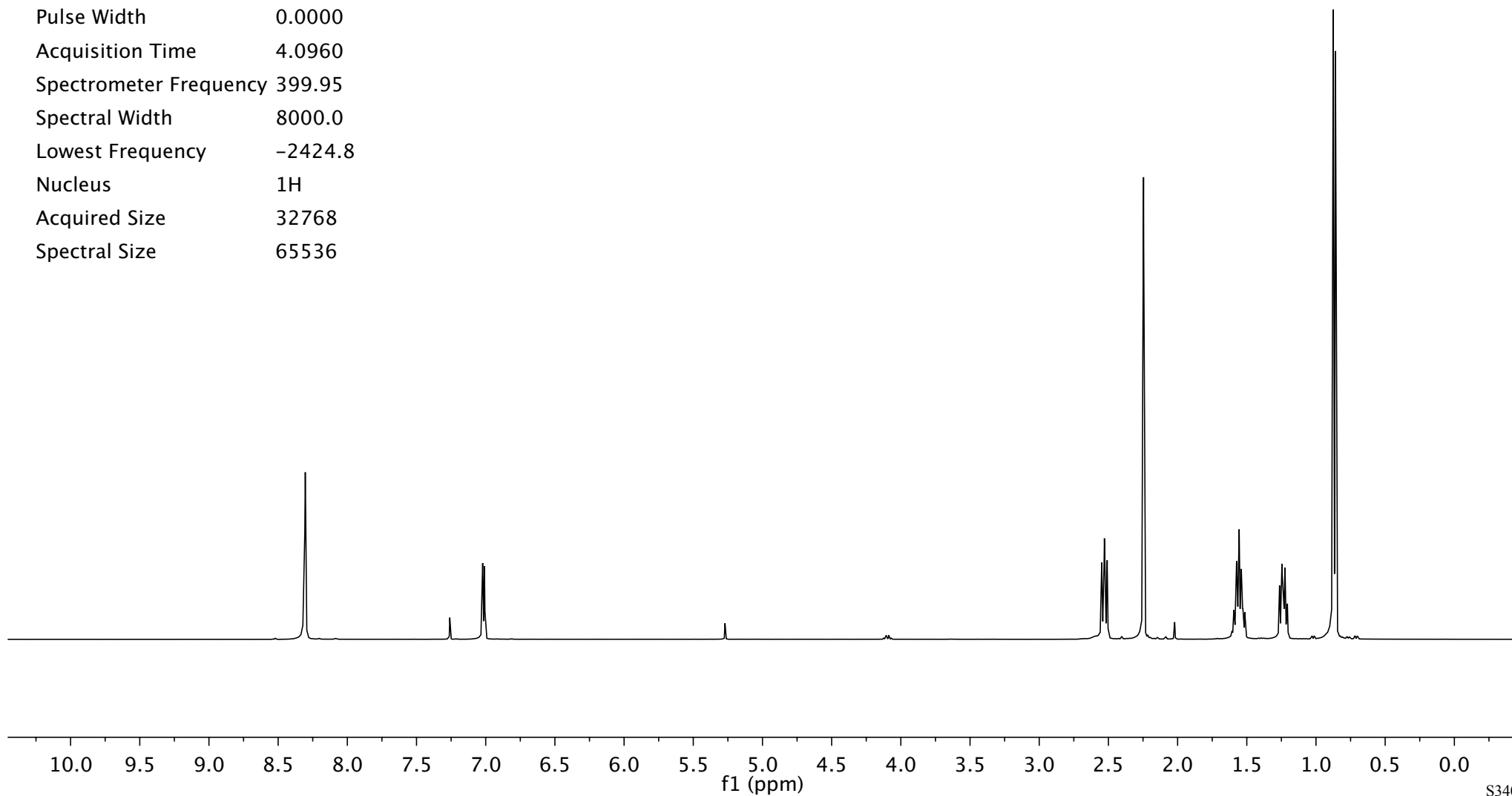
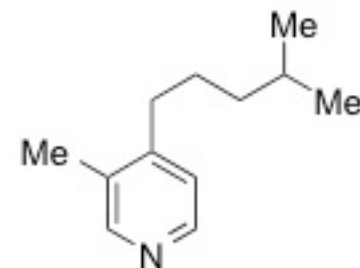


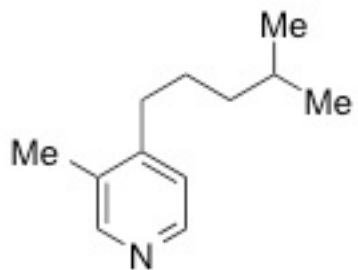


~150.09
 ~147.30
 ~138.11
 ~135.91
 —123.36
 77.41 CDCl₃
 77.16 CDCl₃
 76.90 CDCl₃
 ~38.55
 ~33.40
 ~29.14
 ~27.97
 ~22.69



Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	40
Relaxation Delay	5.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	399.95
Spectral Width	8000.0
Lowest Frequency	-2424.8
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



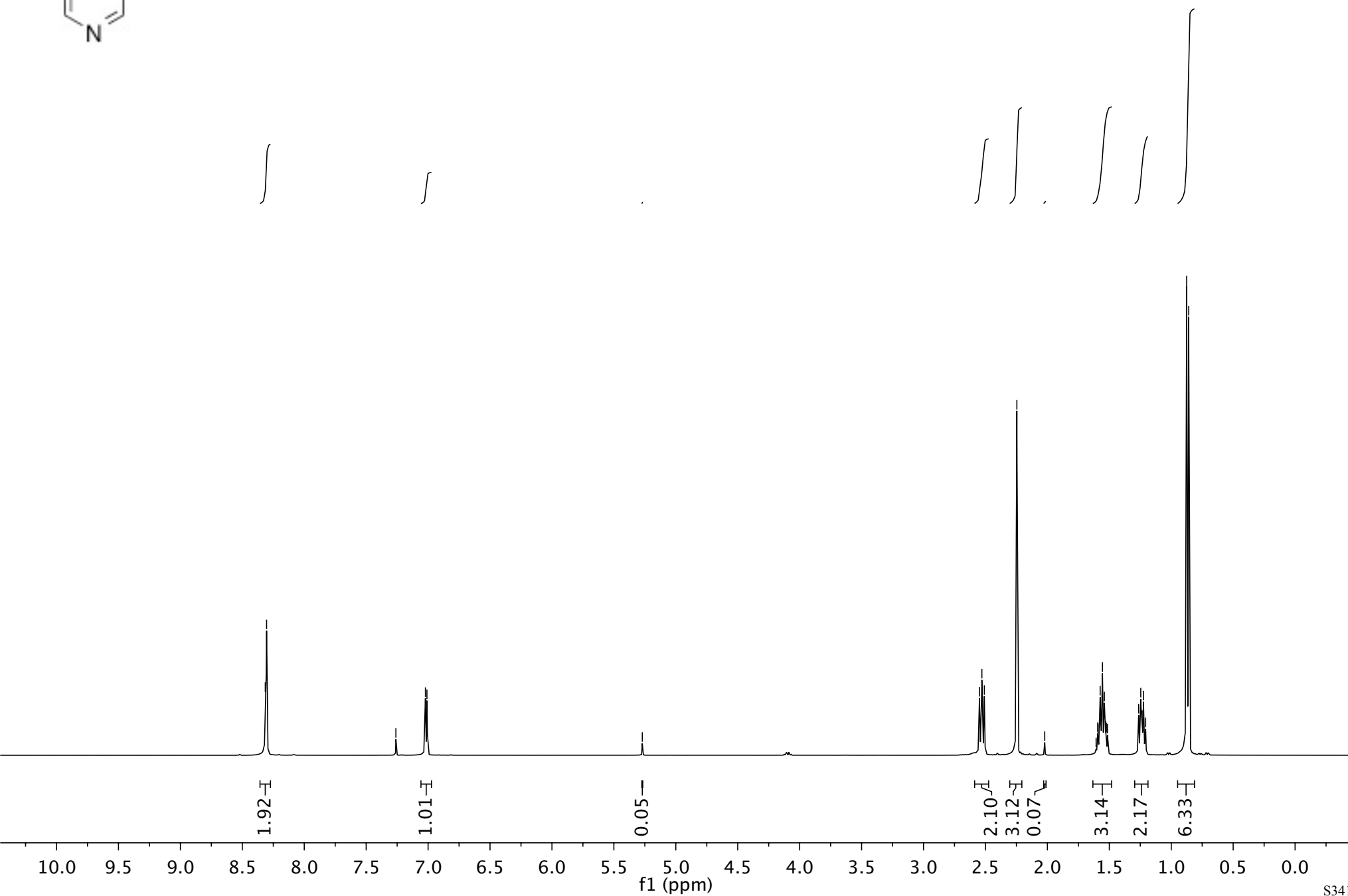


8.31
8.30

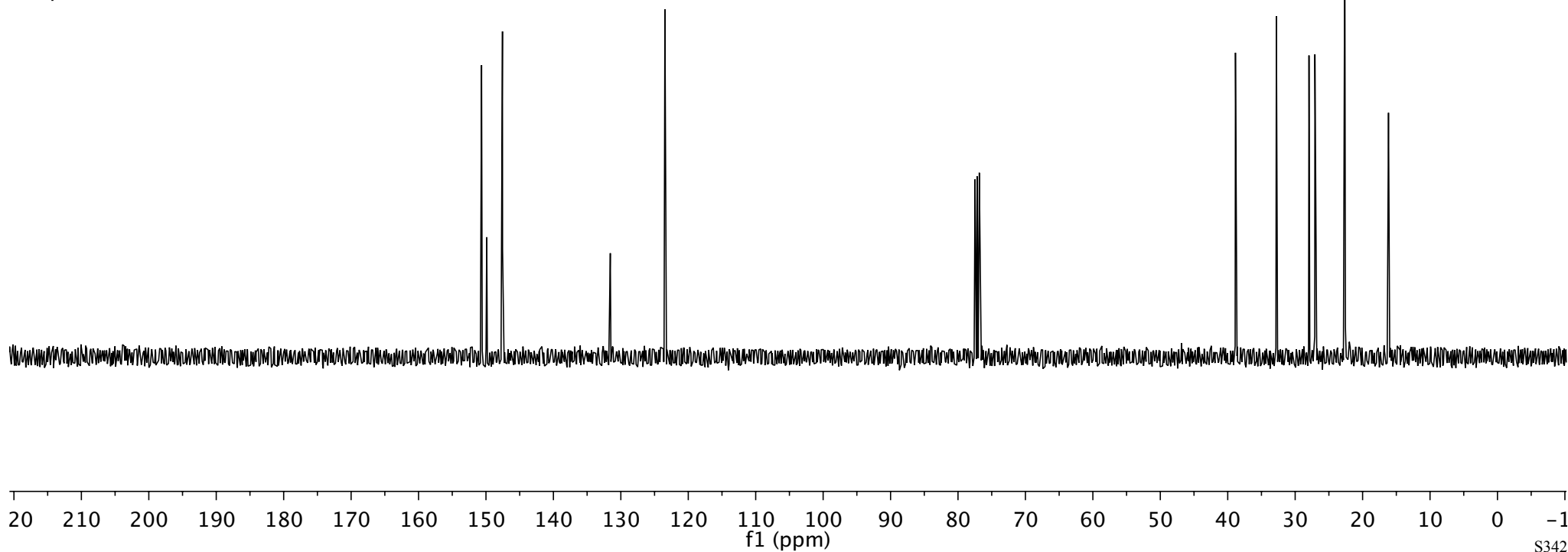
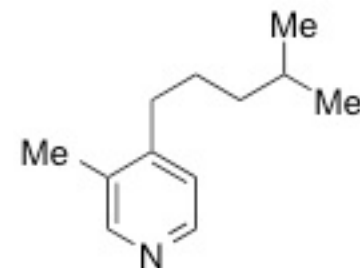
7.26 CDCl₃
7.02
7.01

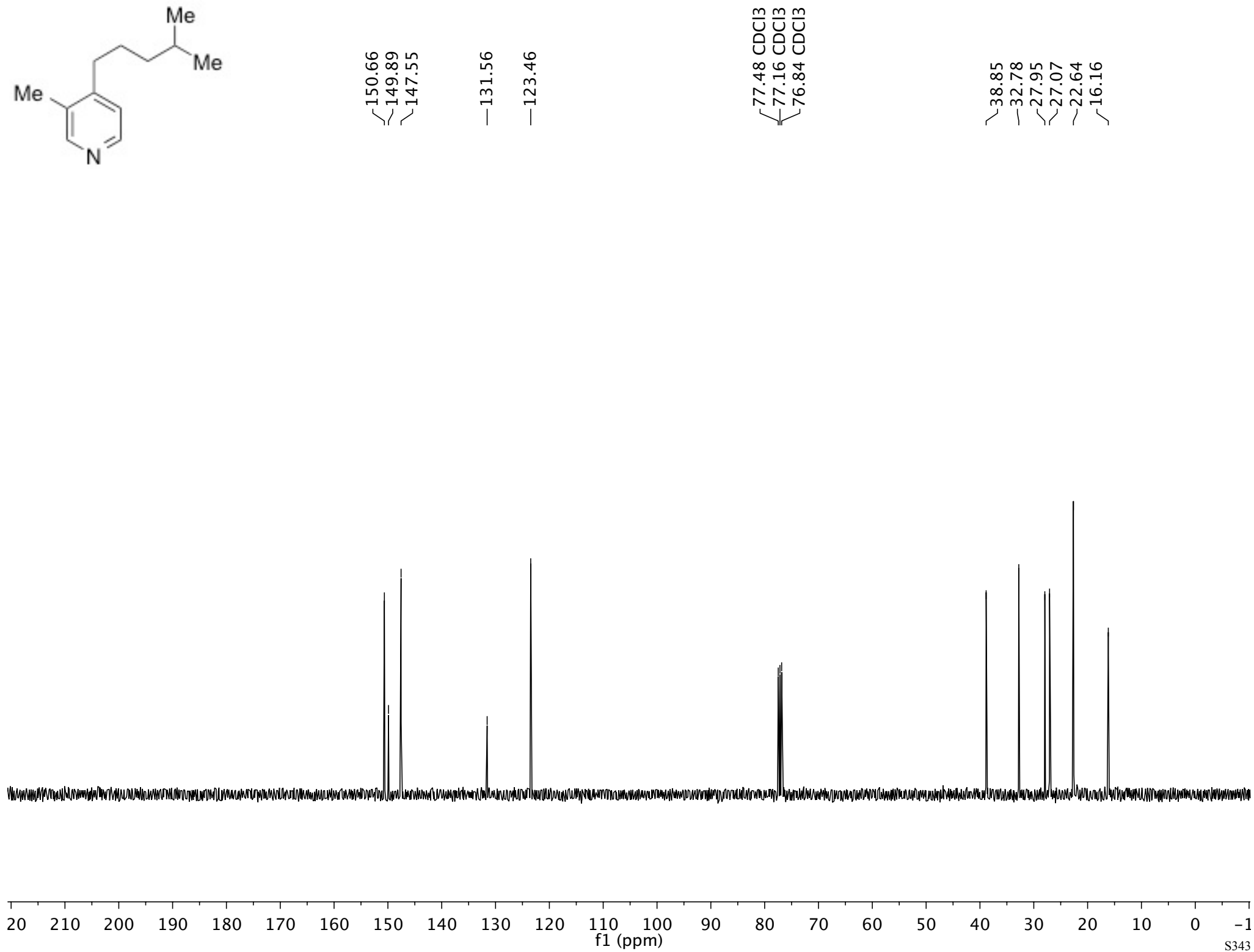
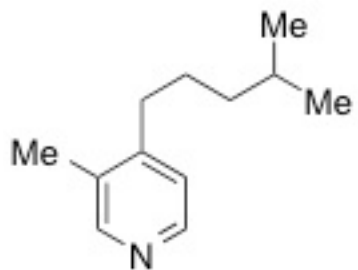
5.27

2.55
2.53
2.51
2.25
2.02
1.61
1.59
1.59
1.58
1.57
1.57
1.56
1.56
1.55
1.54
1.53
1.52
1.51
1.26
1.25
1.24
1.22
1.21
0.88
0.86

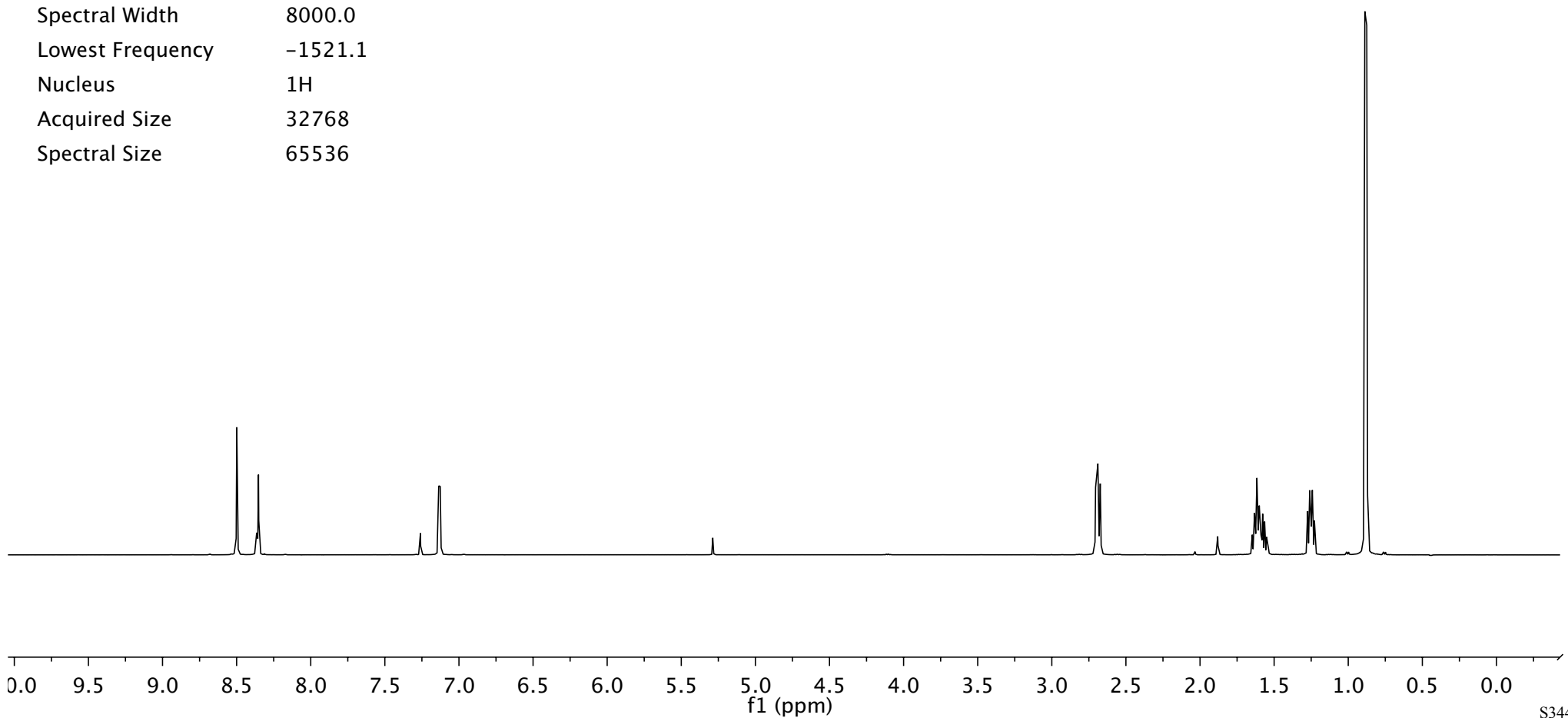
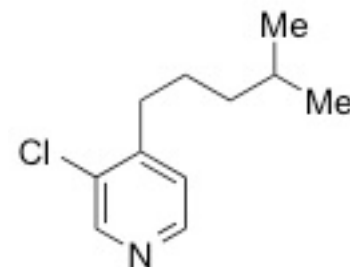


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.3107
Spectrometer Frequency	100.58
Spectral Width	25000.0
Lowest Frequency	-1029.5
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

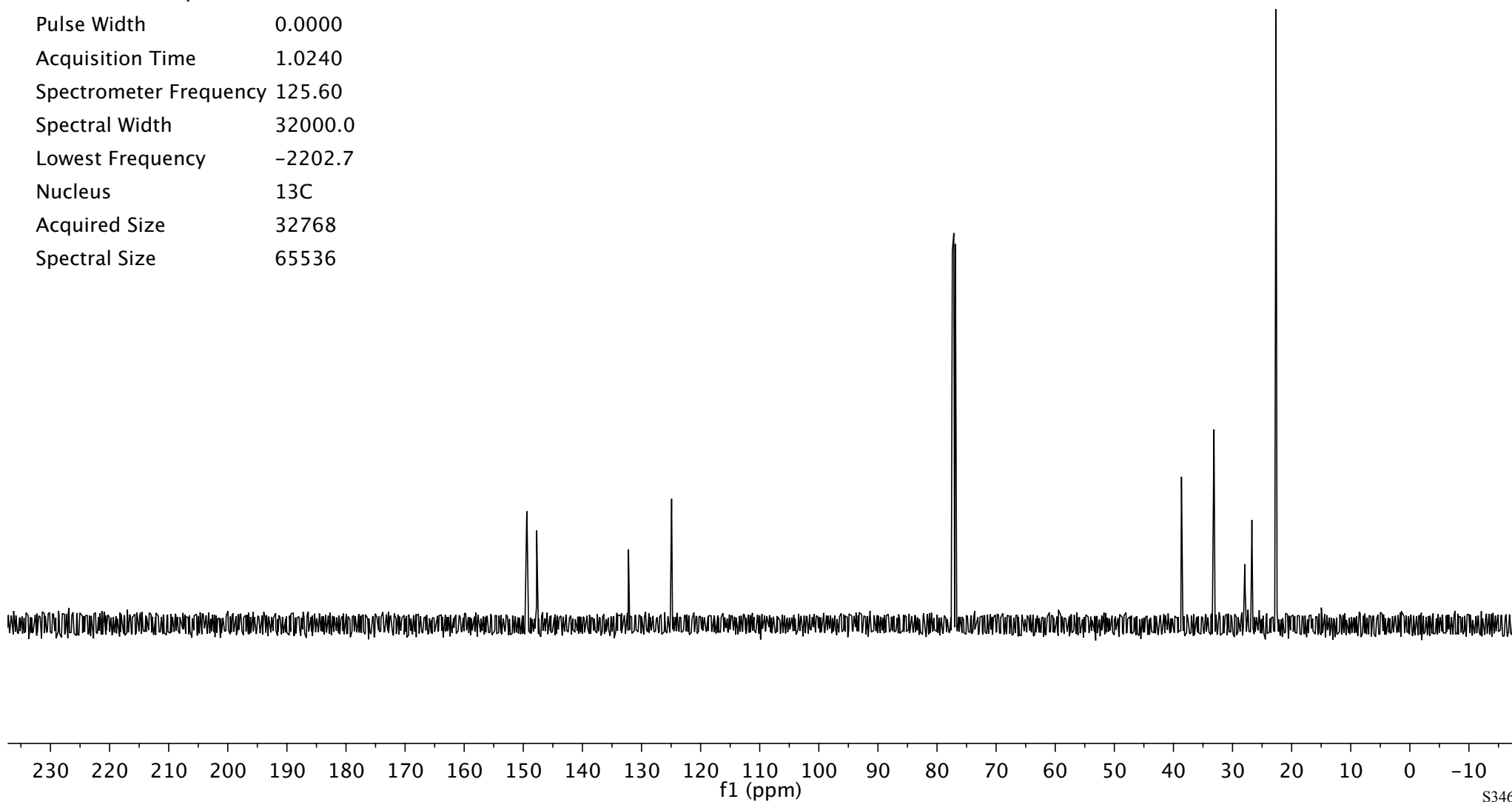
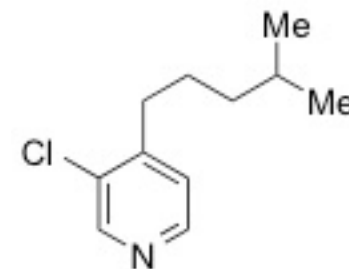


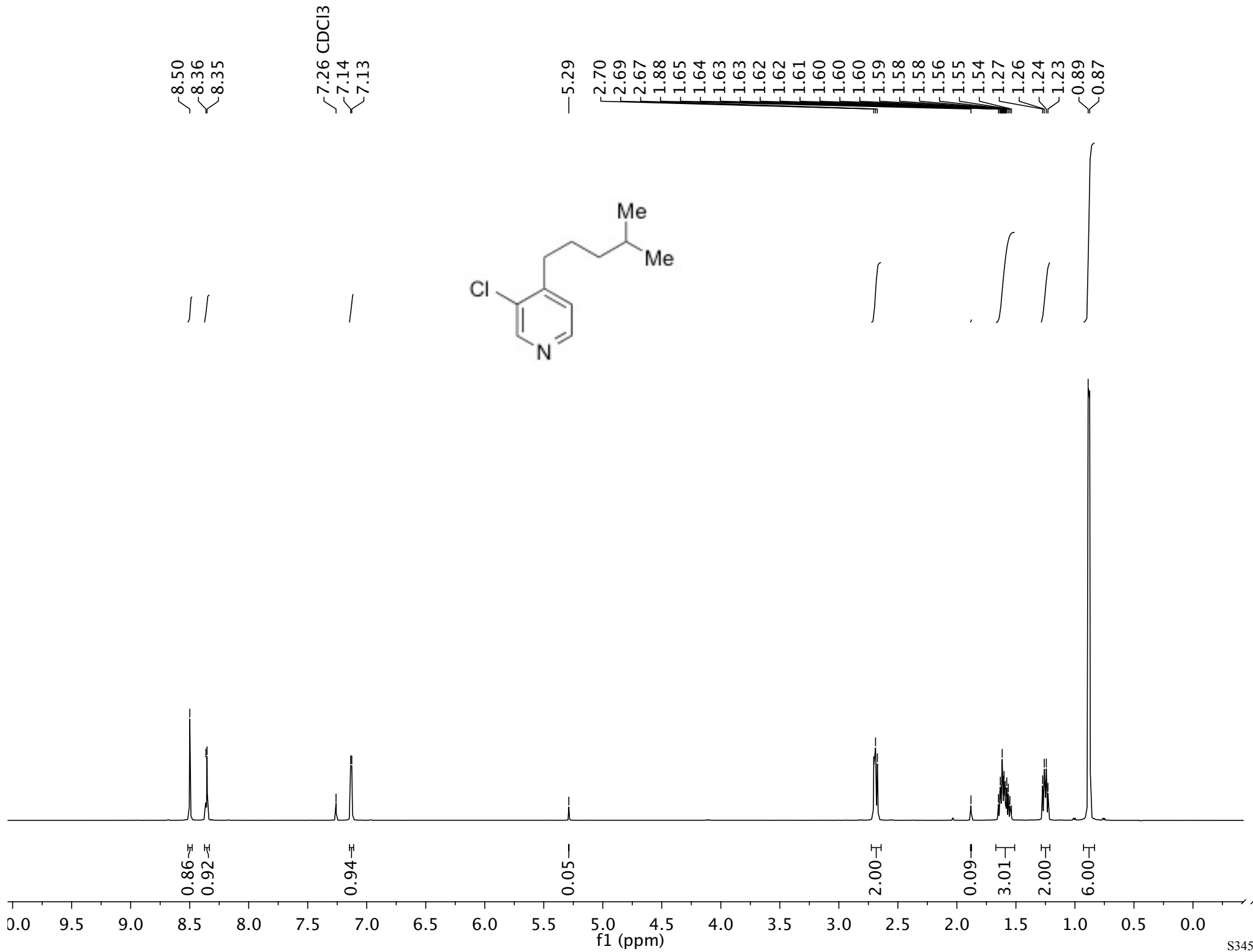


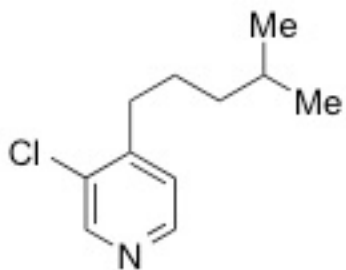
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	26
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2202.7
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536







149.41
149.22
147.72

132.21

124.90

77.41 CDCl₃
77.16 CDCl₃
76.90 CDCl₃

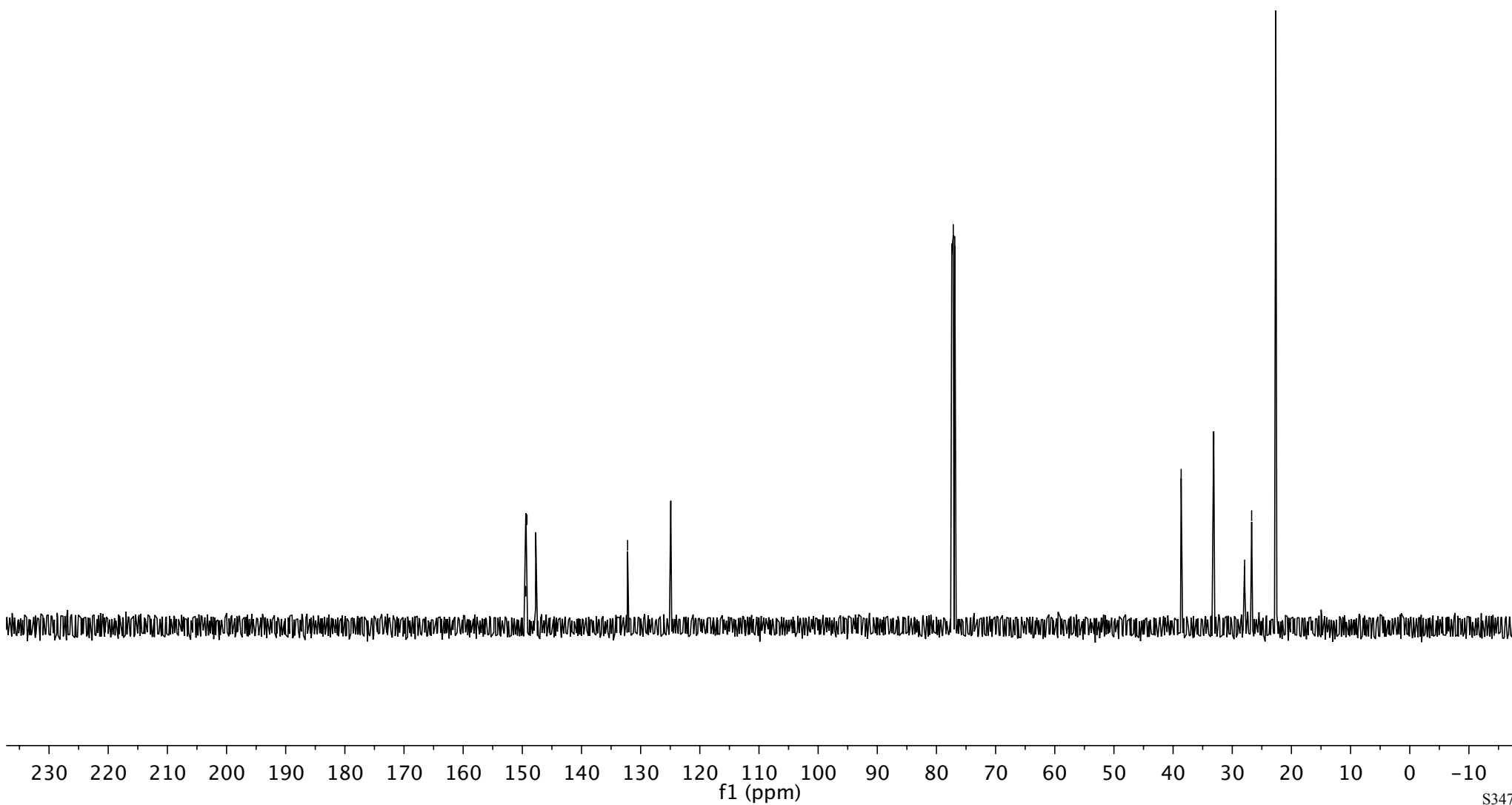
38.64

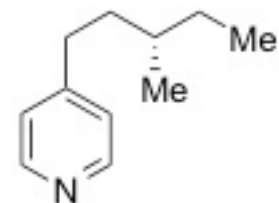
33.14

27.91

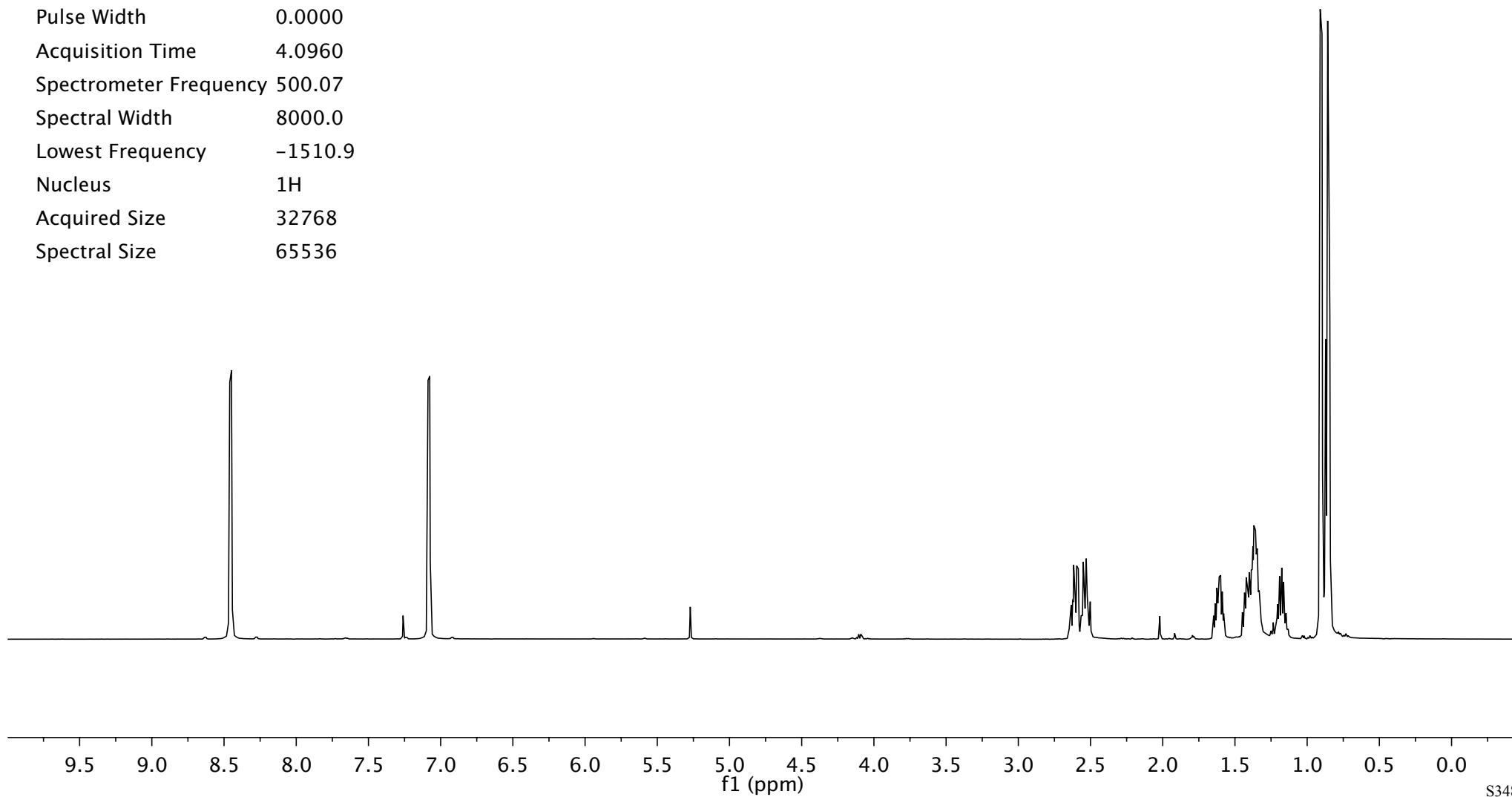
26.73

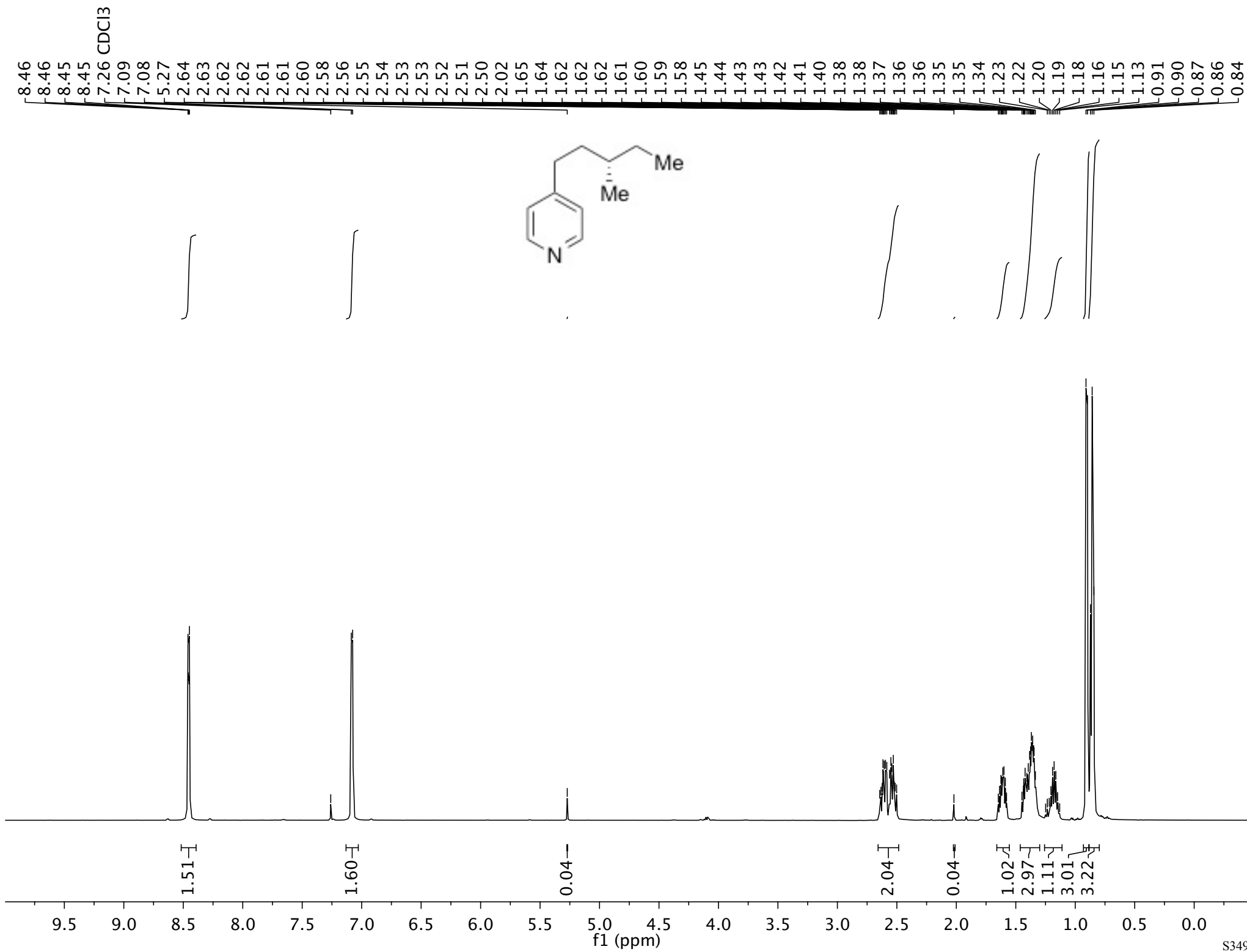
22.64



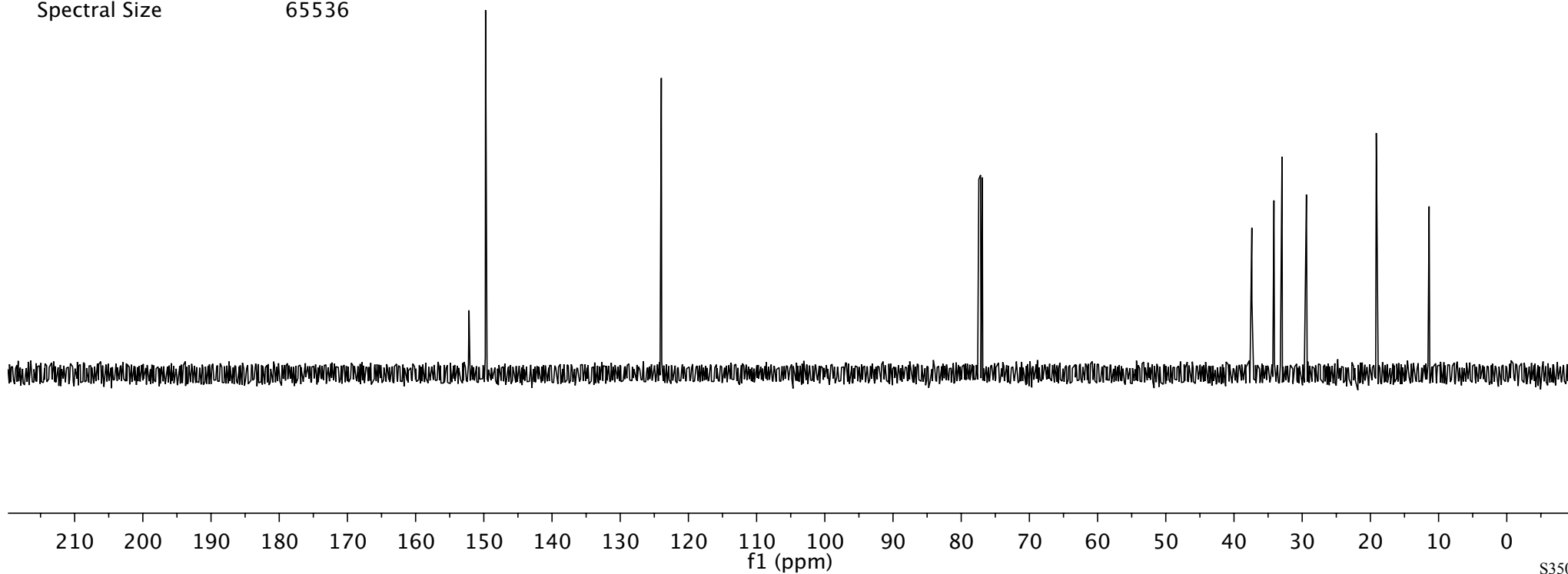
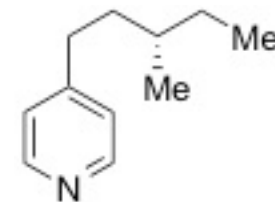


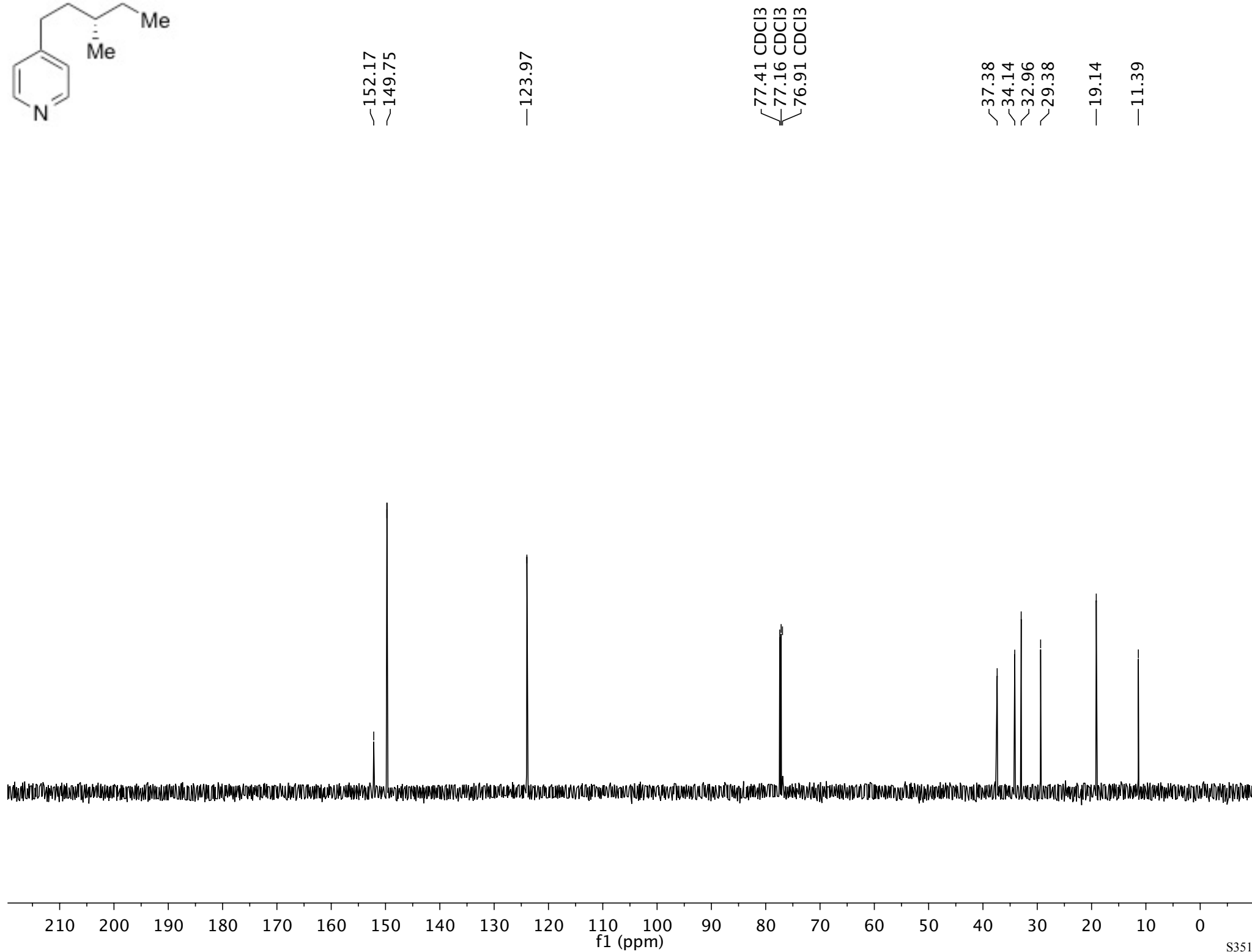
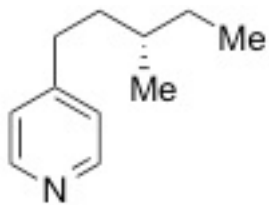
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	22
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1510.9
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

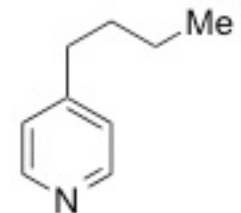




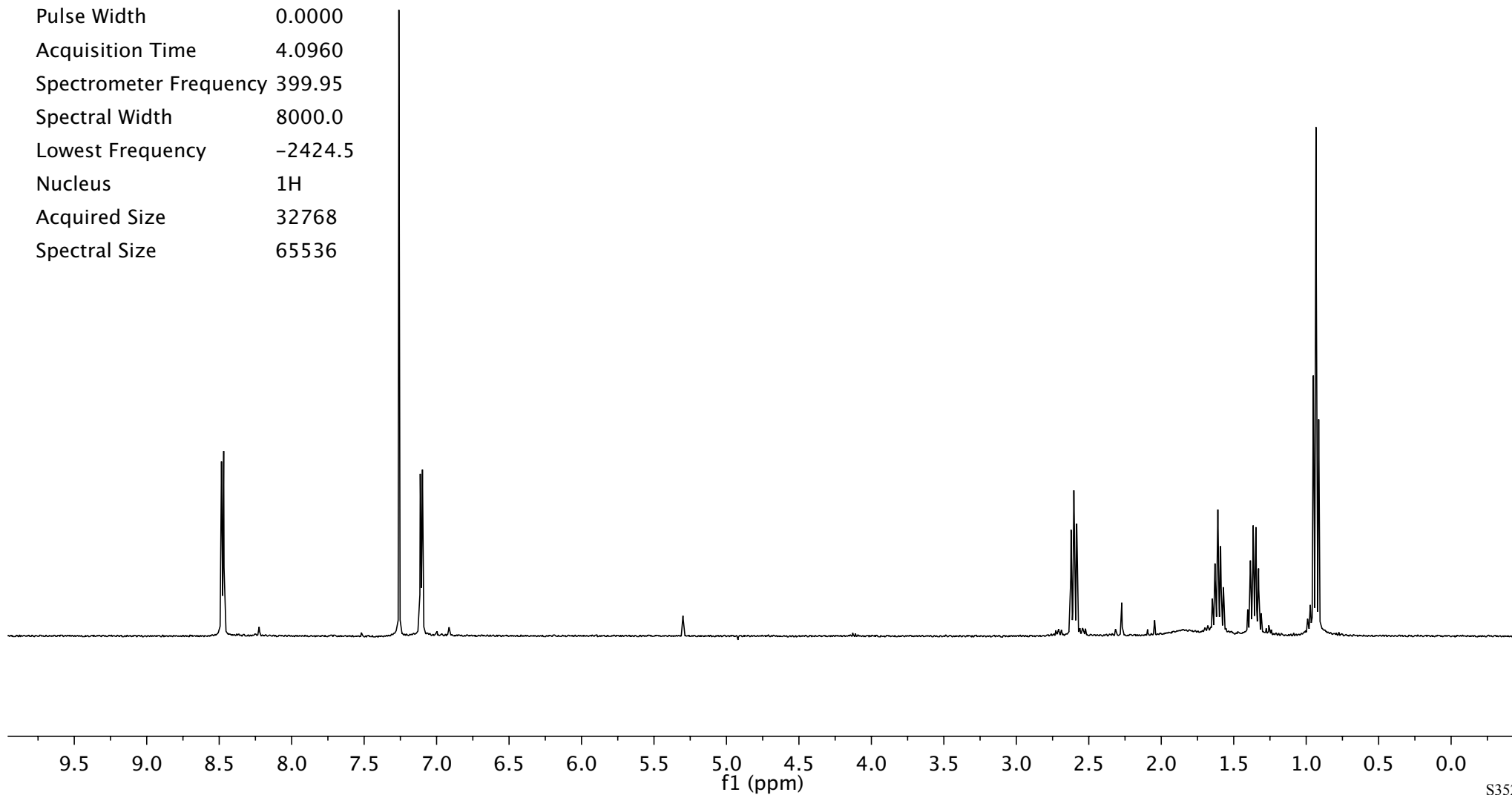
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2204.6
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

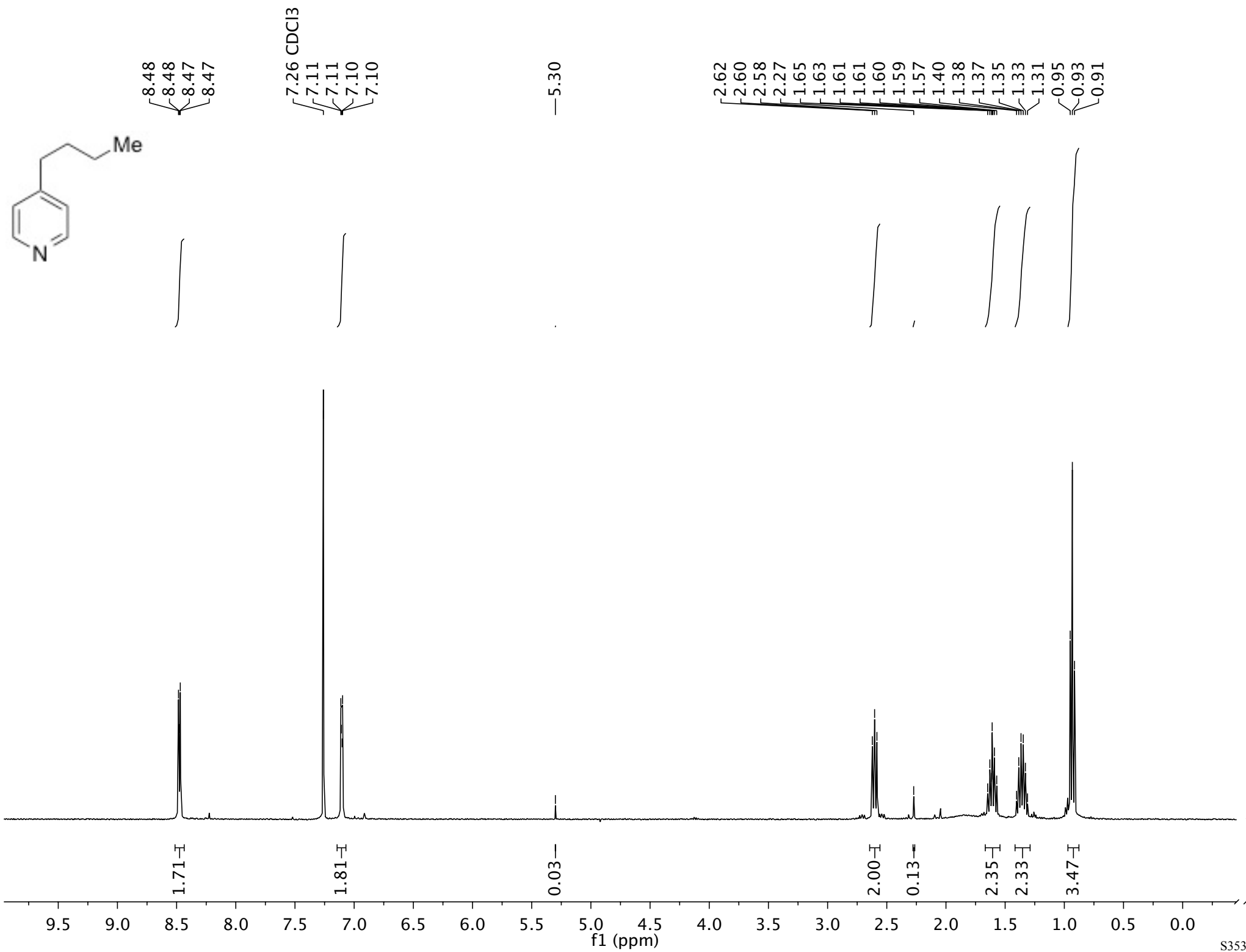




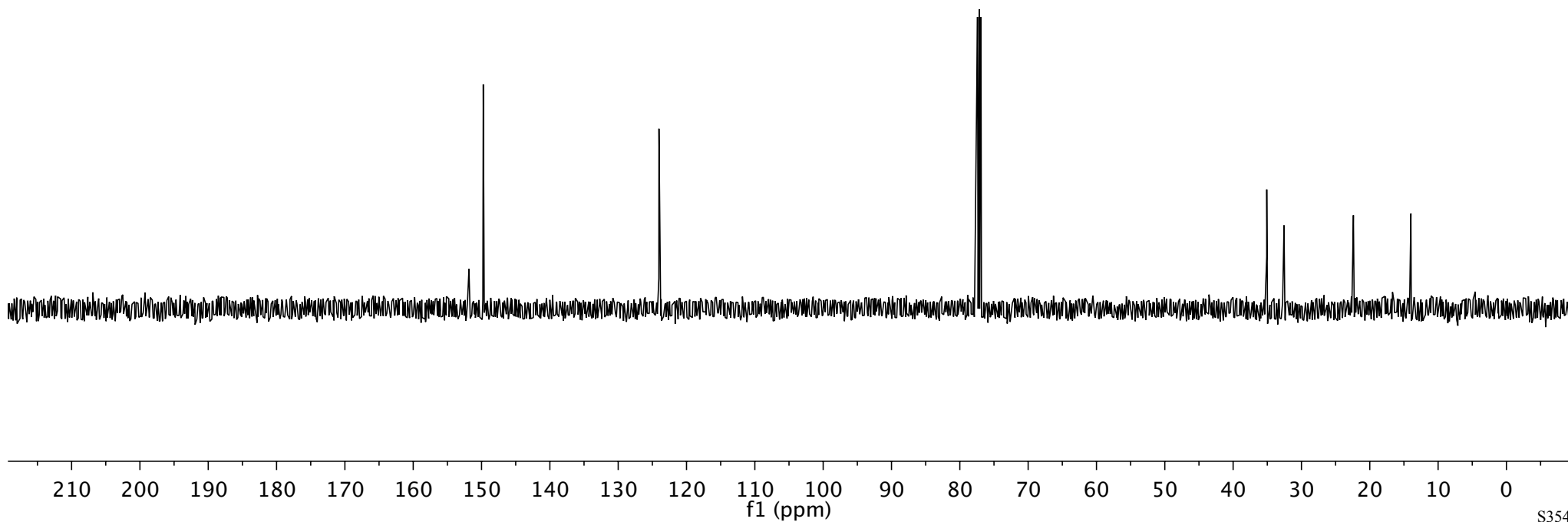
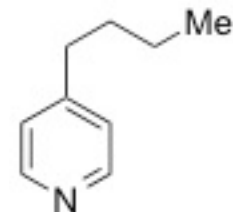


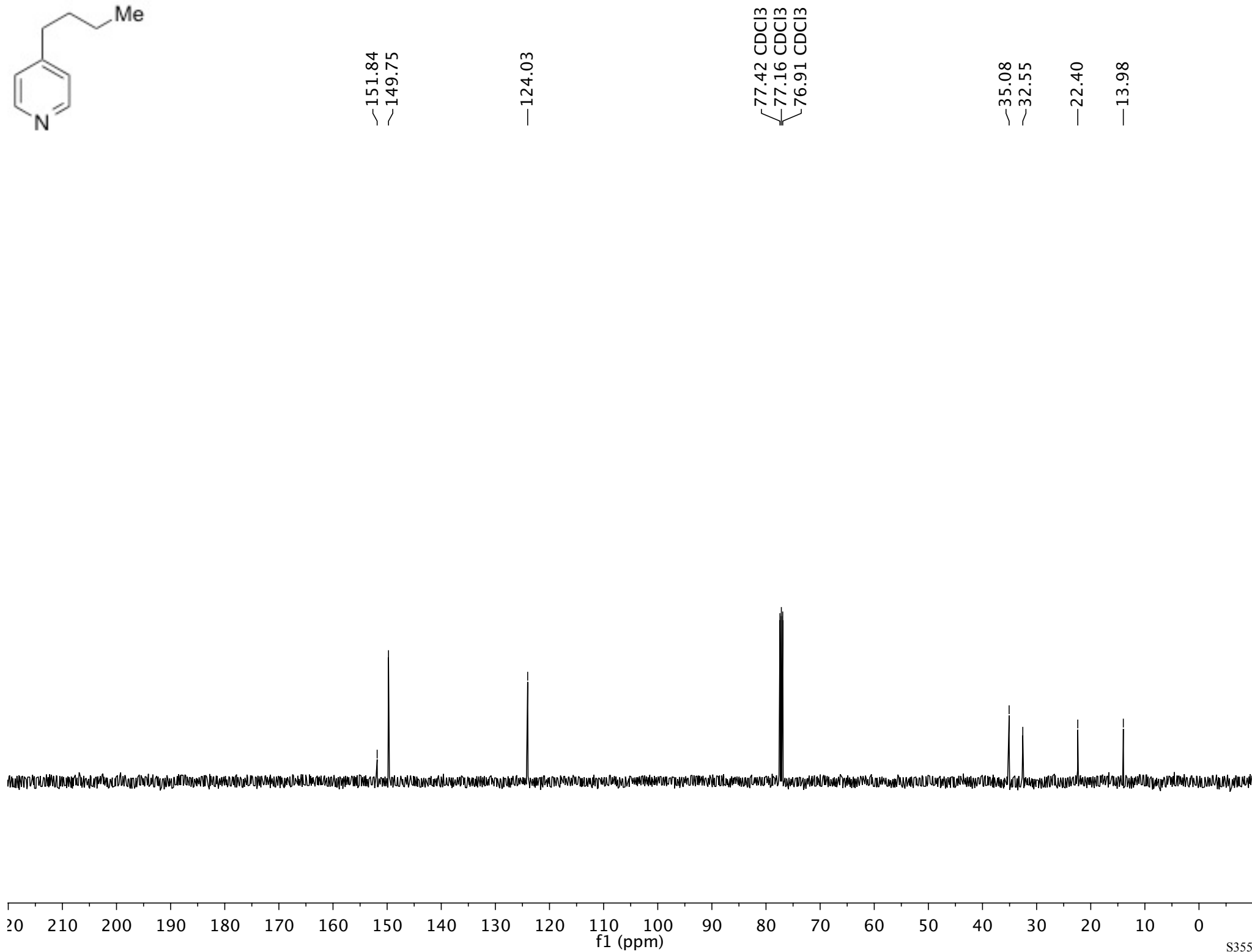
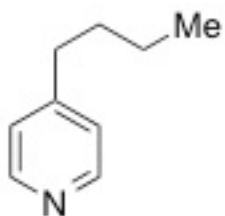
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	399.95
Spectral Width	8000.0
Lowest Frequency	-2424.5
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

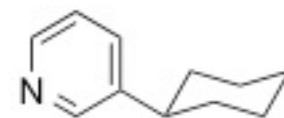




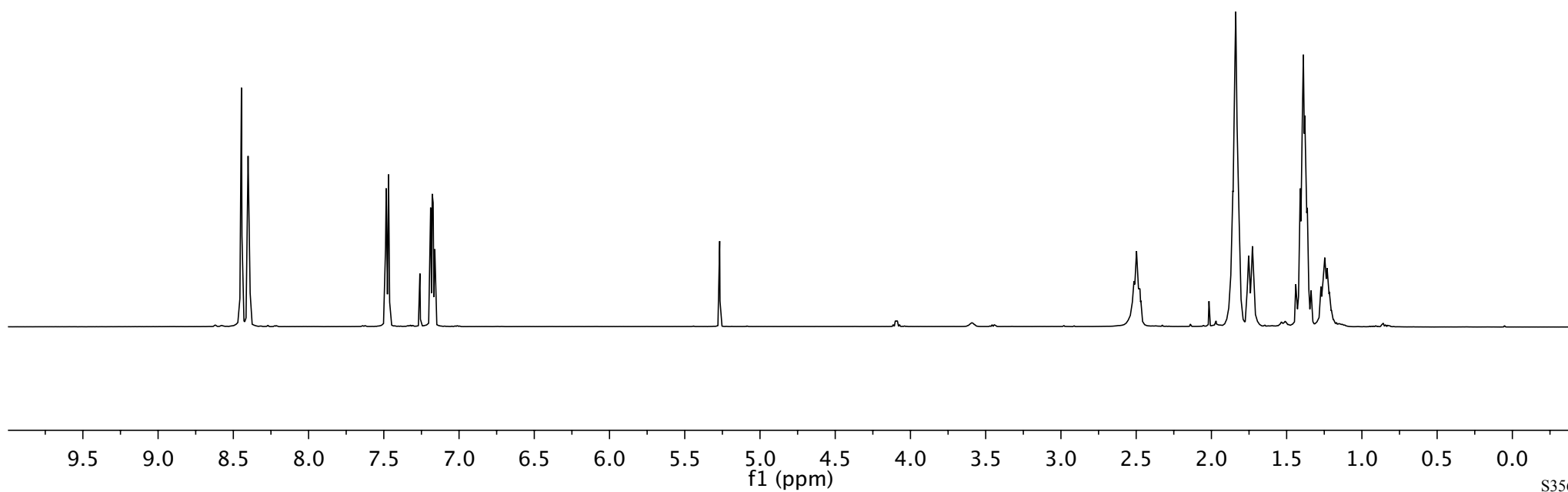
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2199.3
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

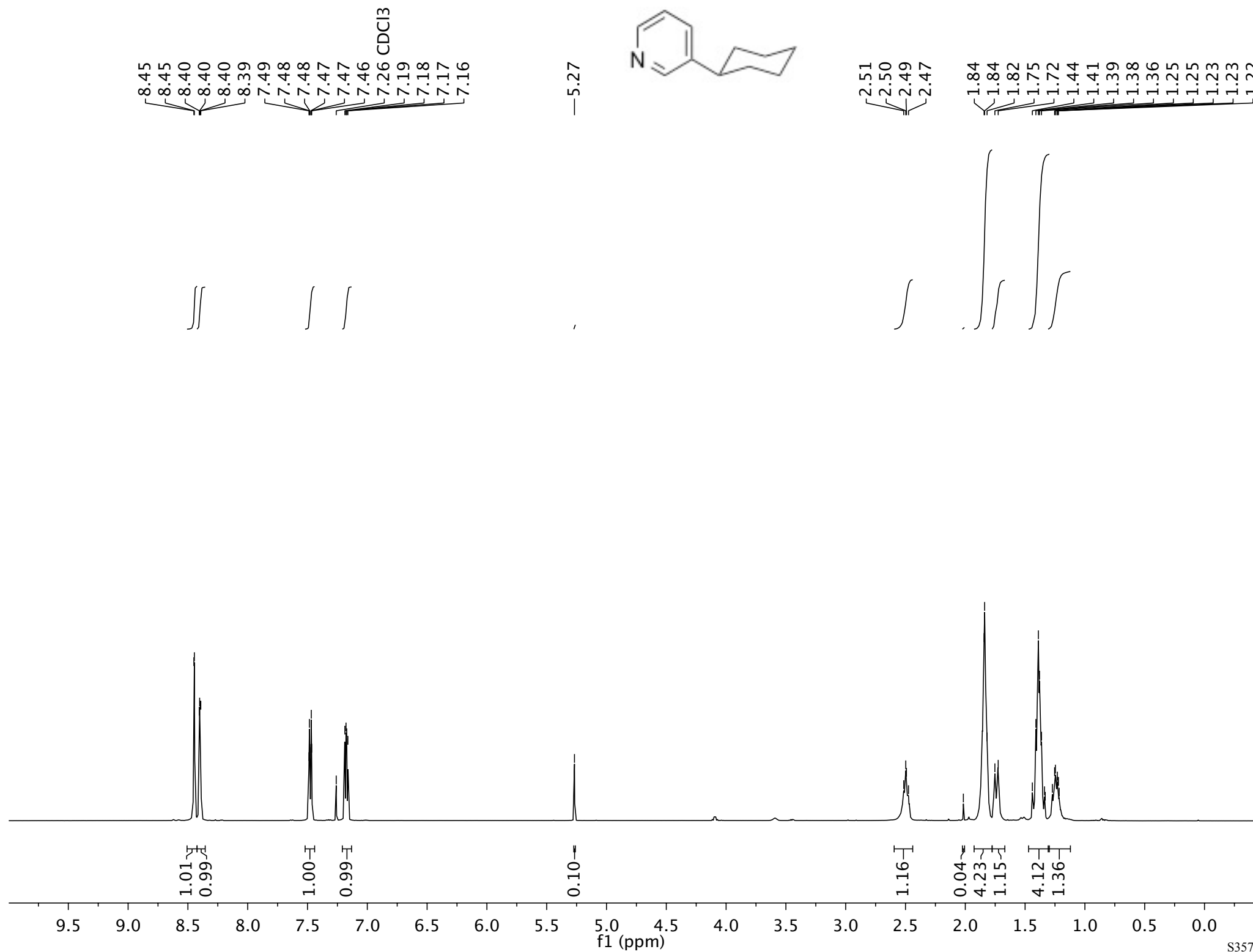




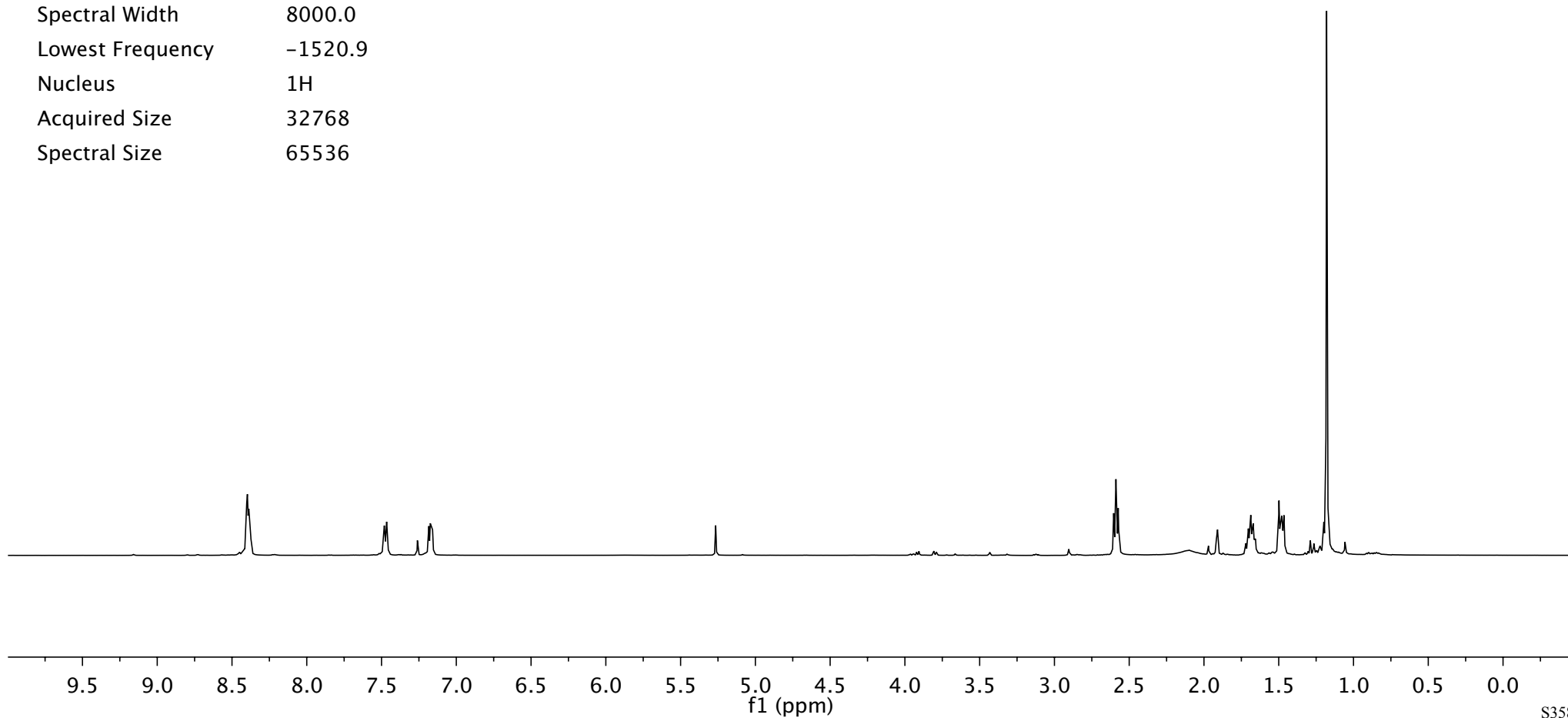
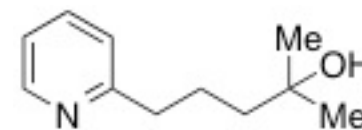


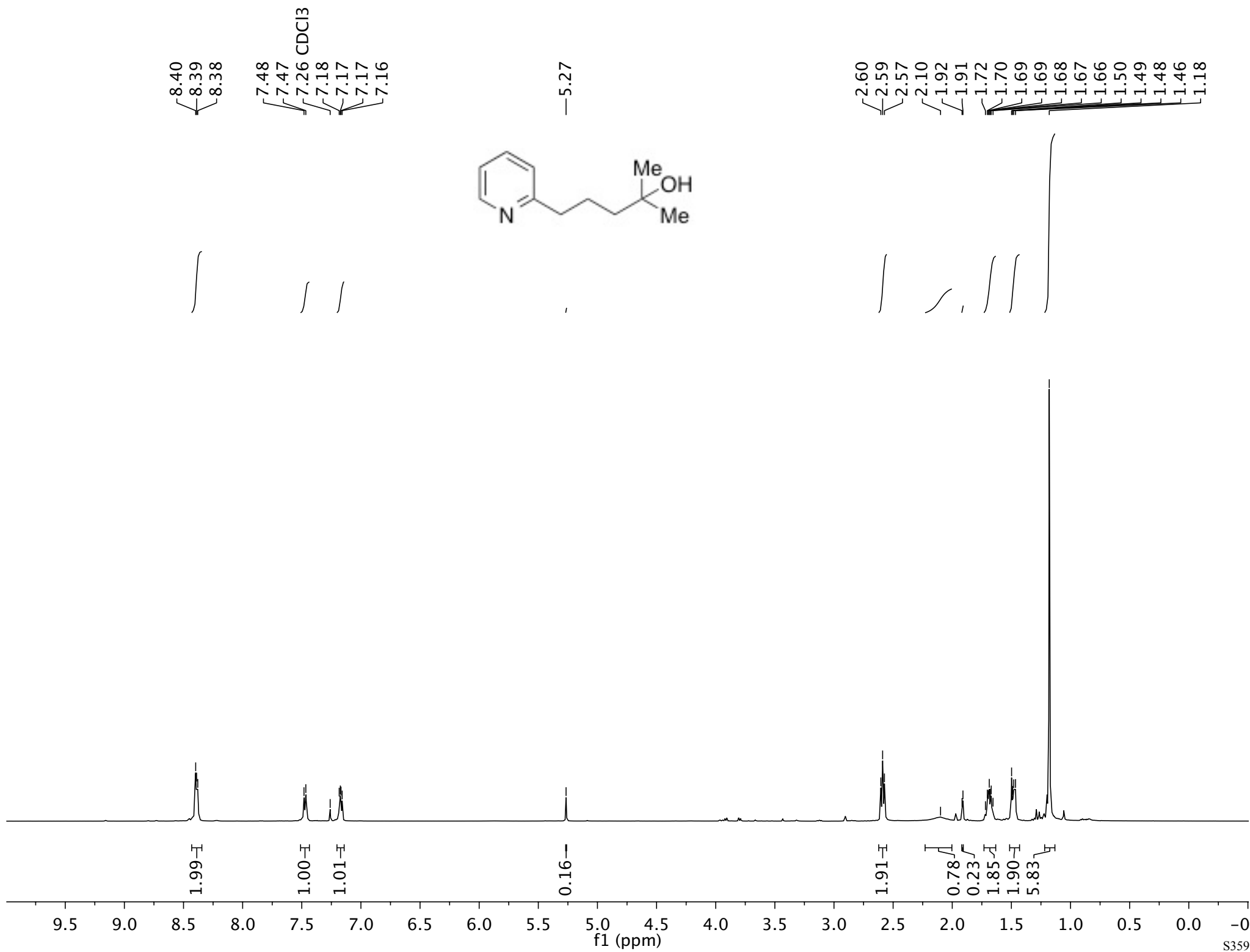
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	22
Relaxation Delay	15.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



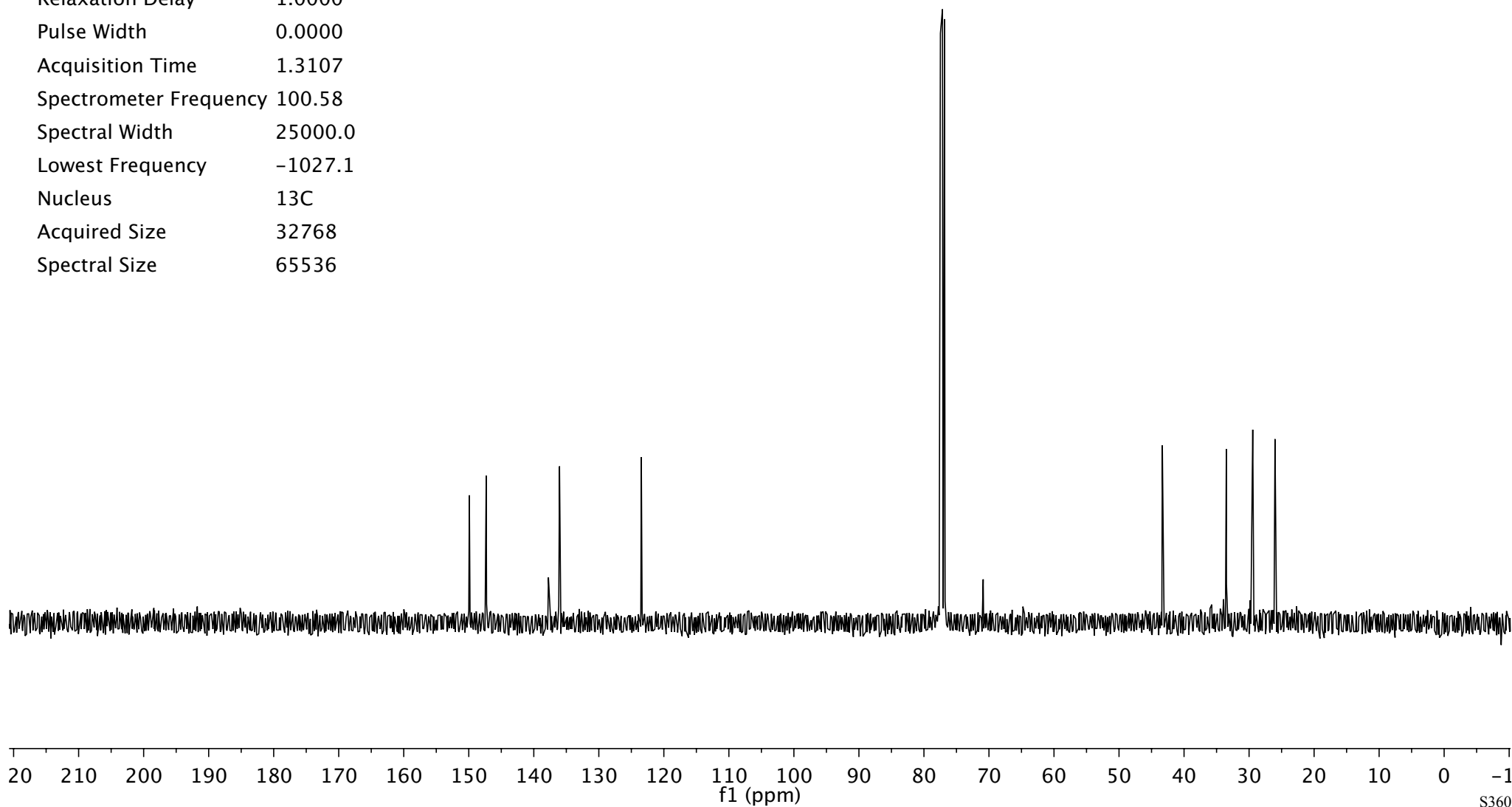
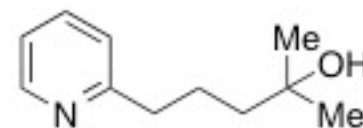


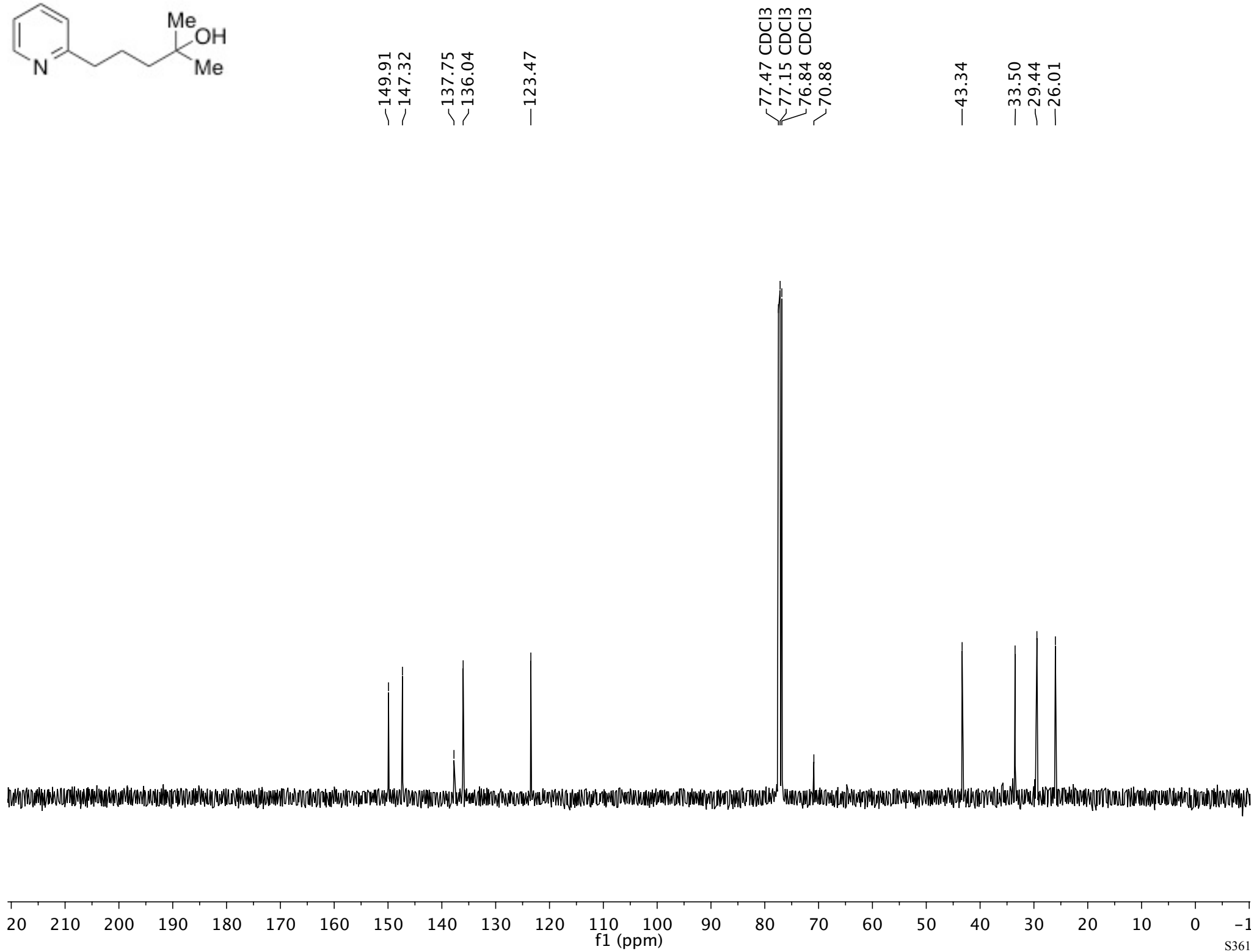
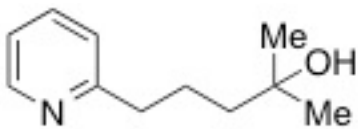
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	22
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1520.9
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

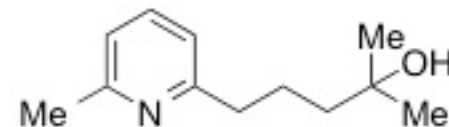




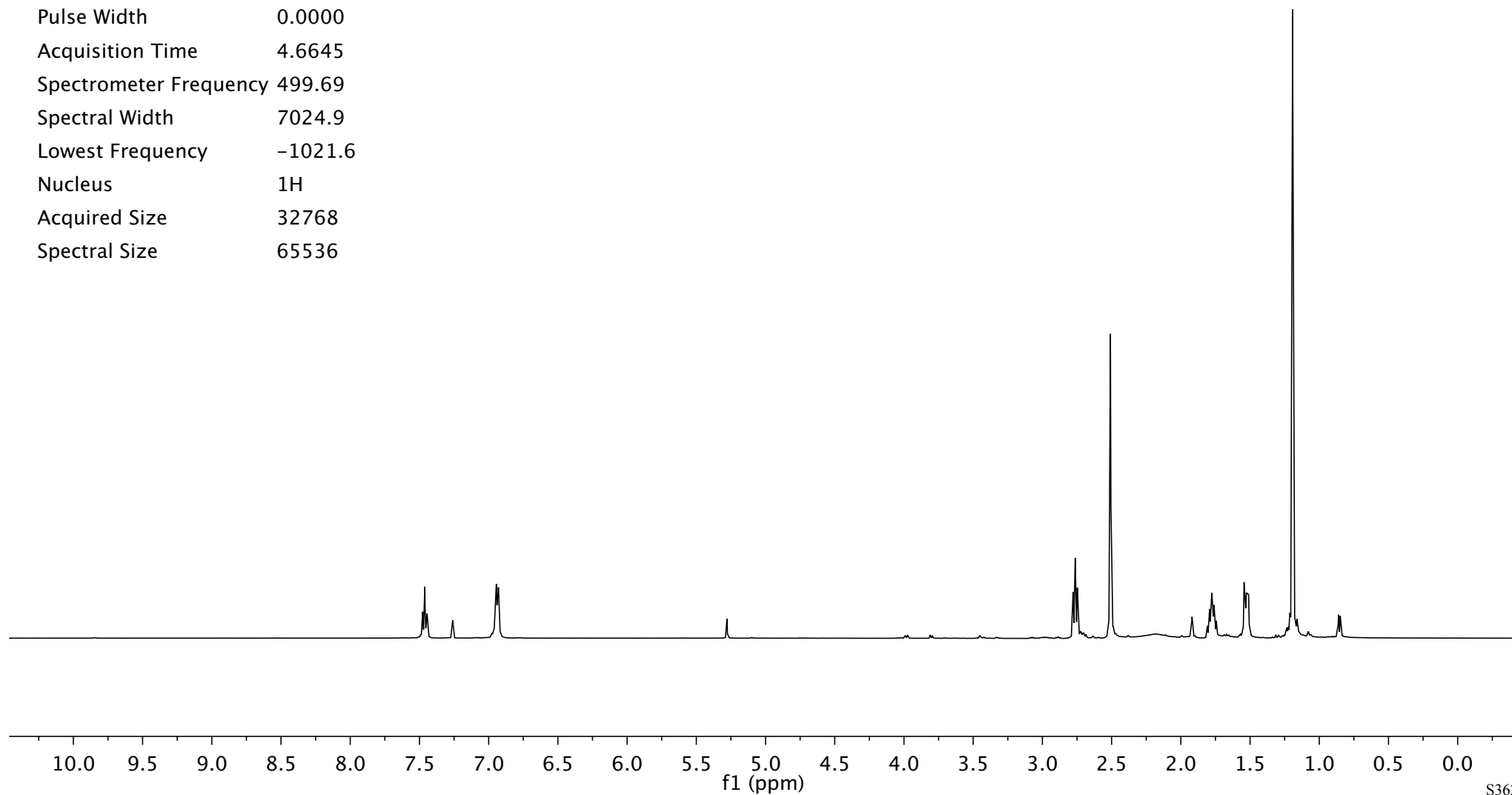
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3107
Spectrometer Frequency	100.58
Spectral Width	25000.0
Lowest Frequency	-1027.1
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

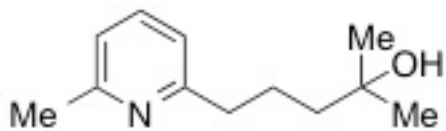






Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	41
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.69
Spectral Width	7024.9
Lowest Frequency	-1021.6
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

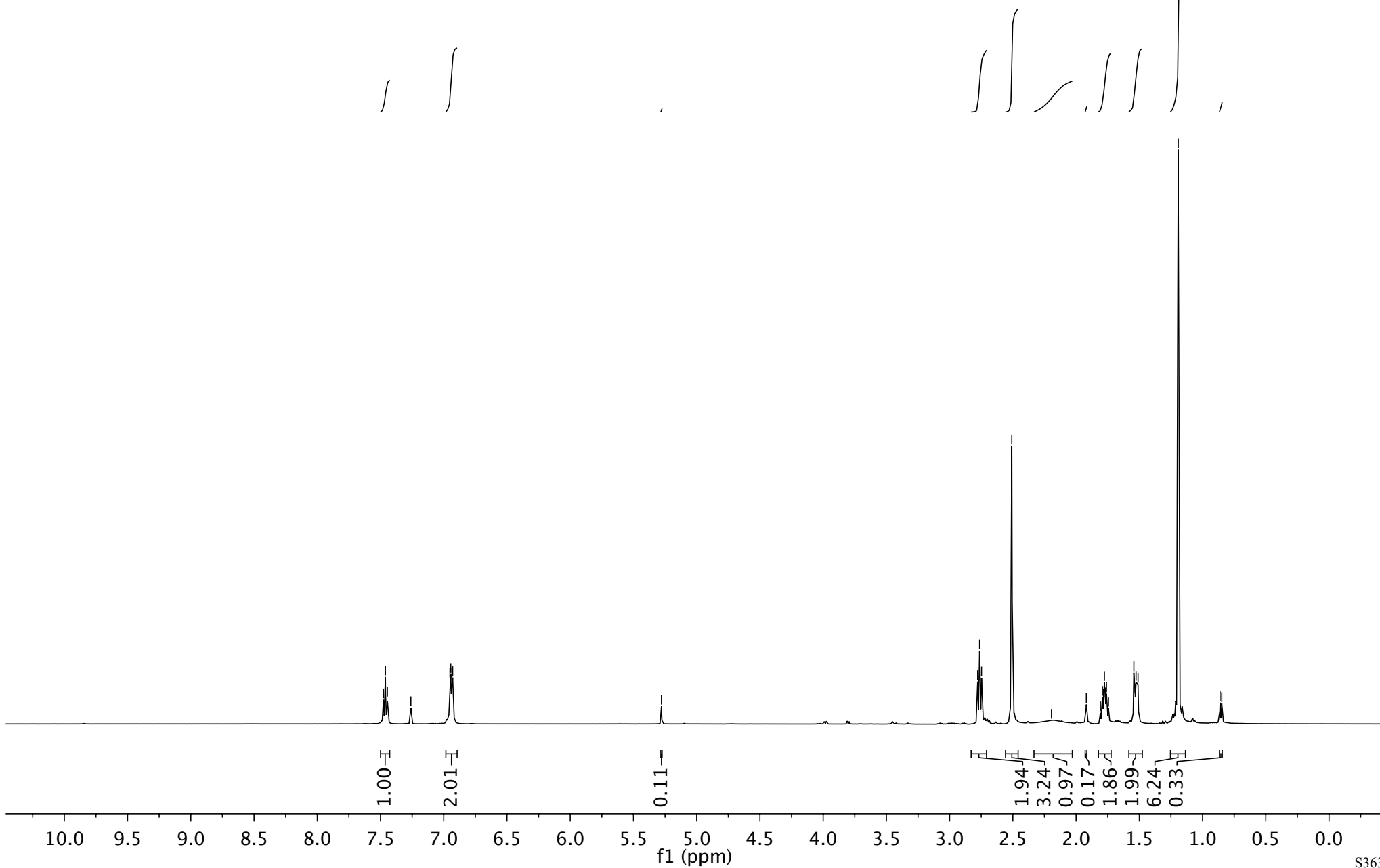


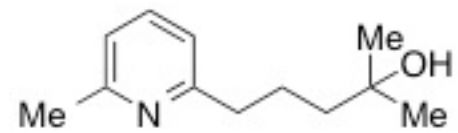


7.48
7.46
7.45
7.26 CDCl₃
6.95
6.94
6.94
6.93

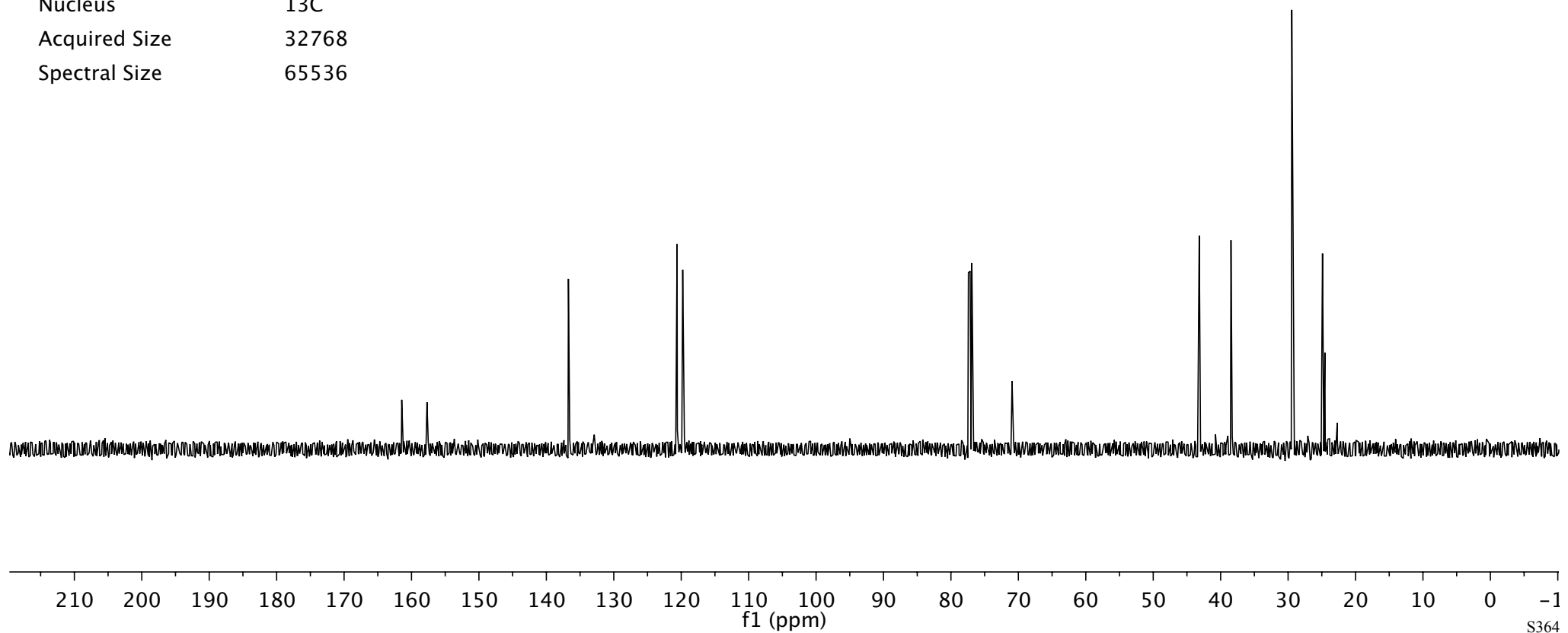
5.28

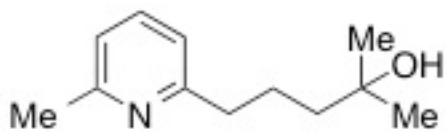
2.78
2.76
2.75
2.51
2.19
1.92
1.81
1.79
1.78
1.78
1.77
1.76
1.74
1.54
1.53
1.53
1.51
1.19
0.86
0.85





Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1276.7
Nucleus	13C
Acquired Size	32768
Spectral Size	65536





—161.45
—157.70

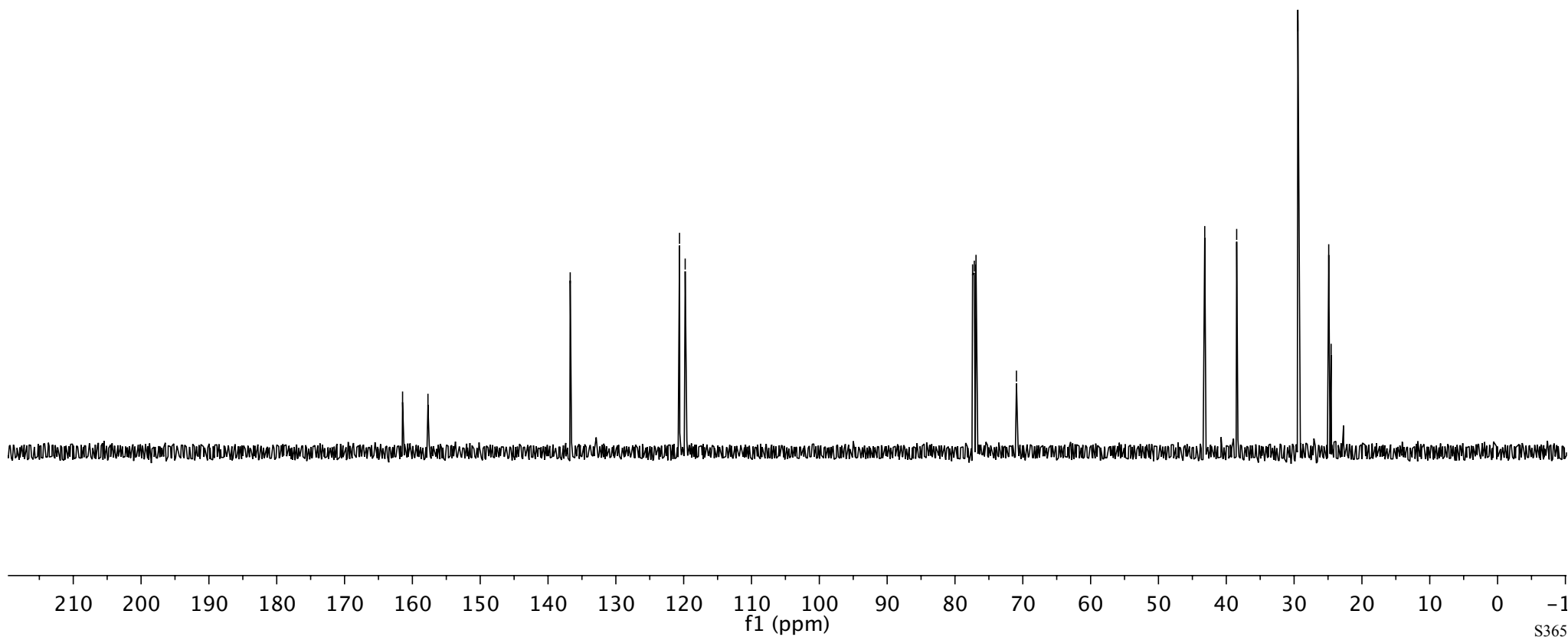
—136.73

—120.61
—119.78

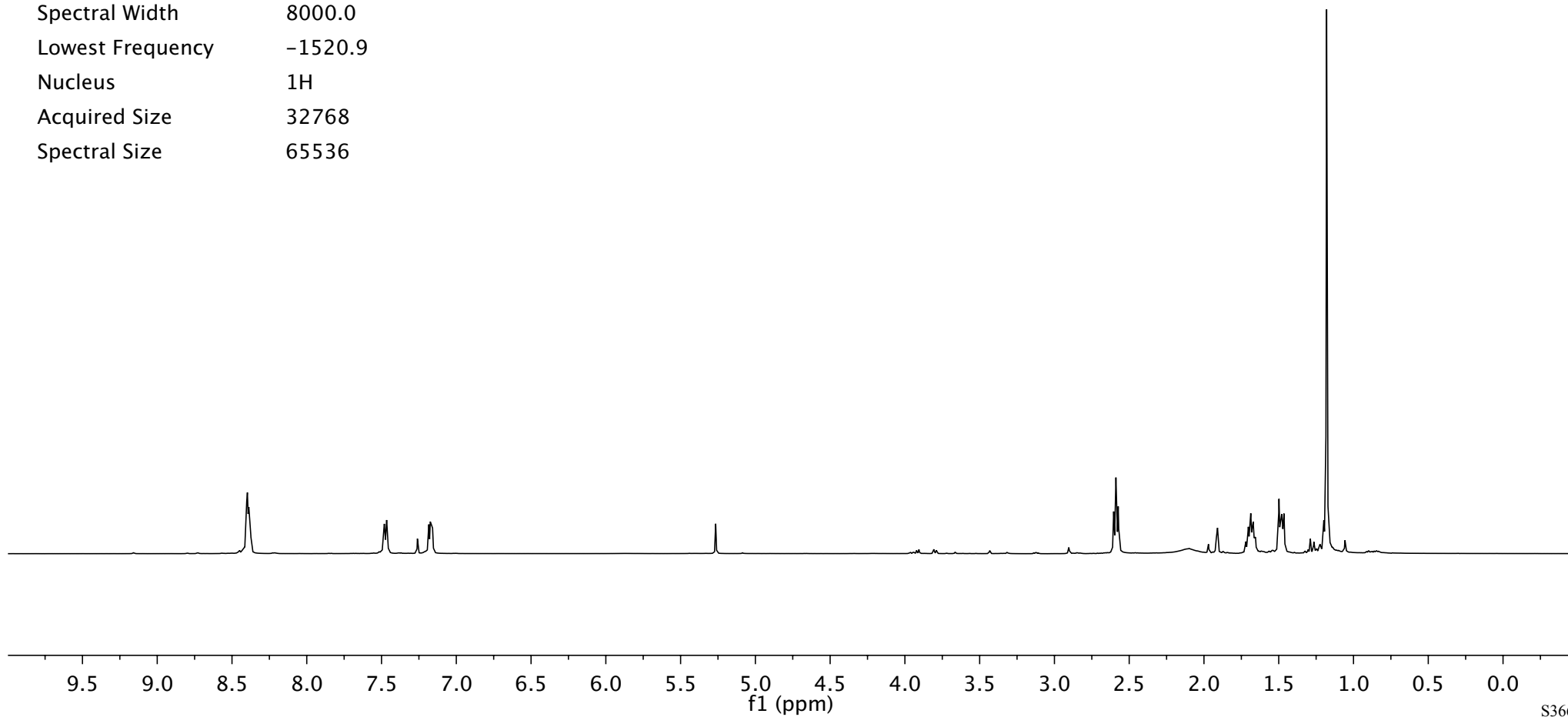
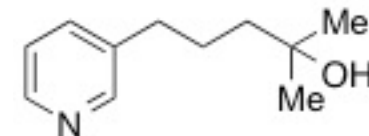
77.41 CDCl₃
77.15 CDCl₃
76.90 CDCl₃
70.94

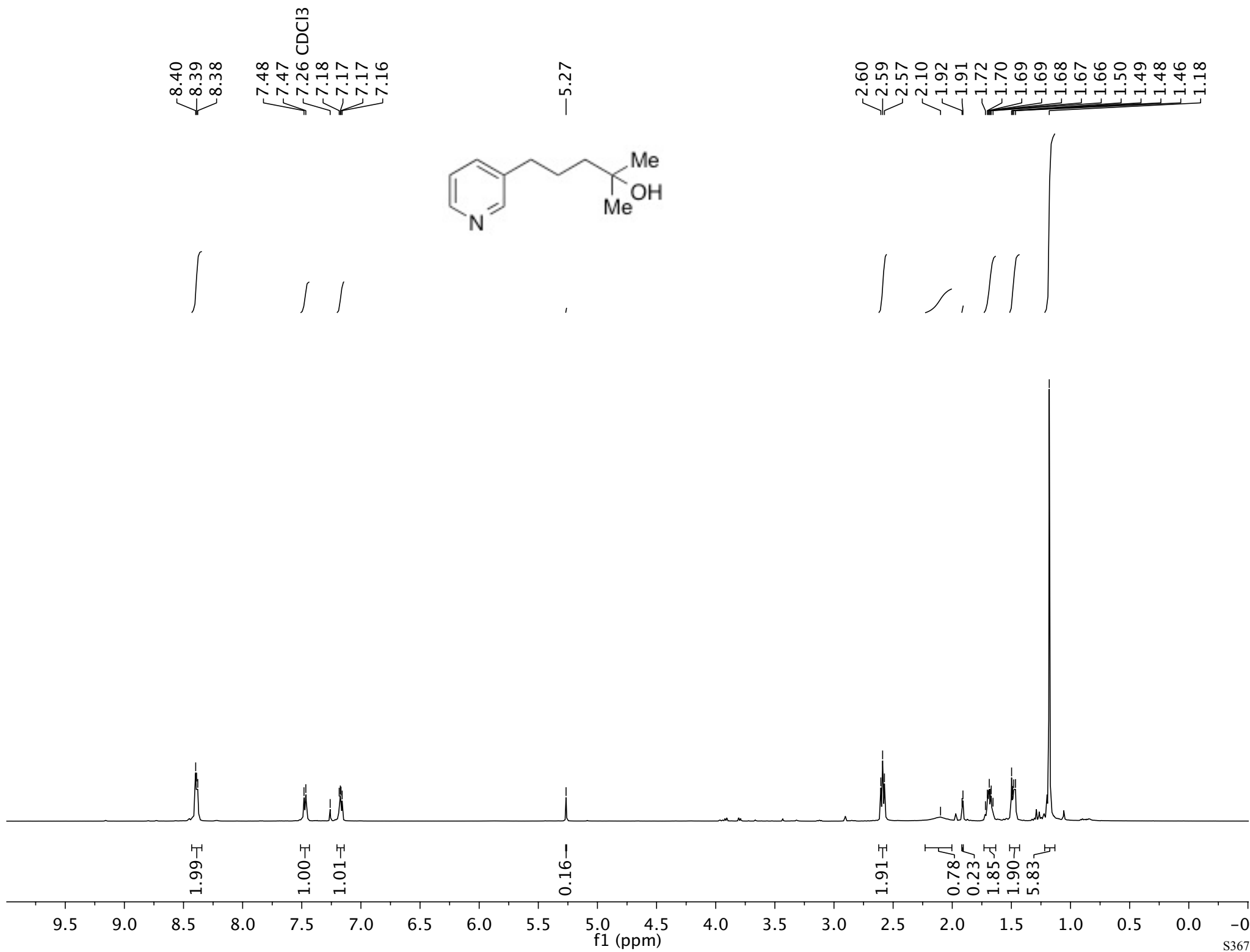
—43.17
—38.47

—29.45
—24.90
—24.54

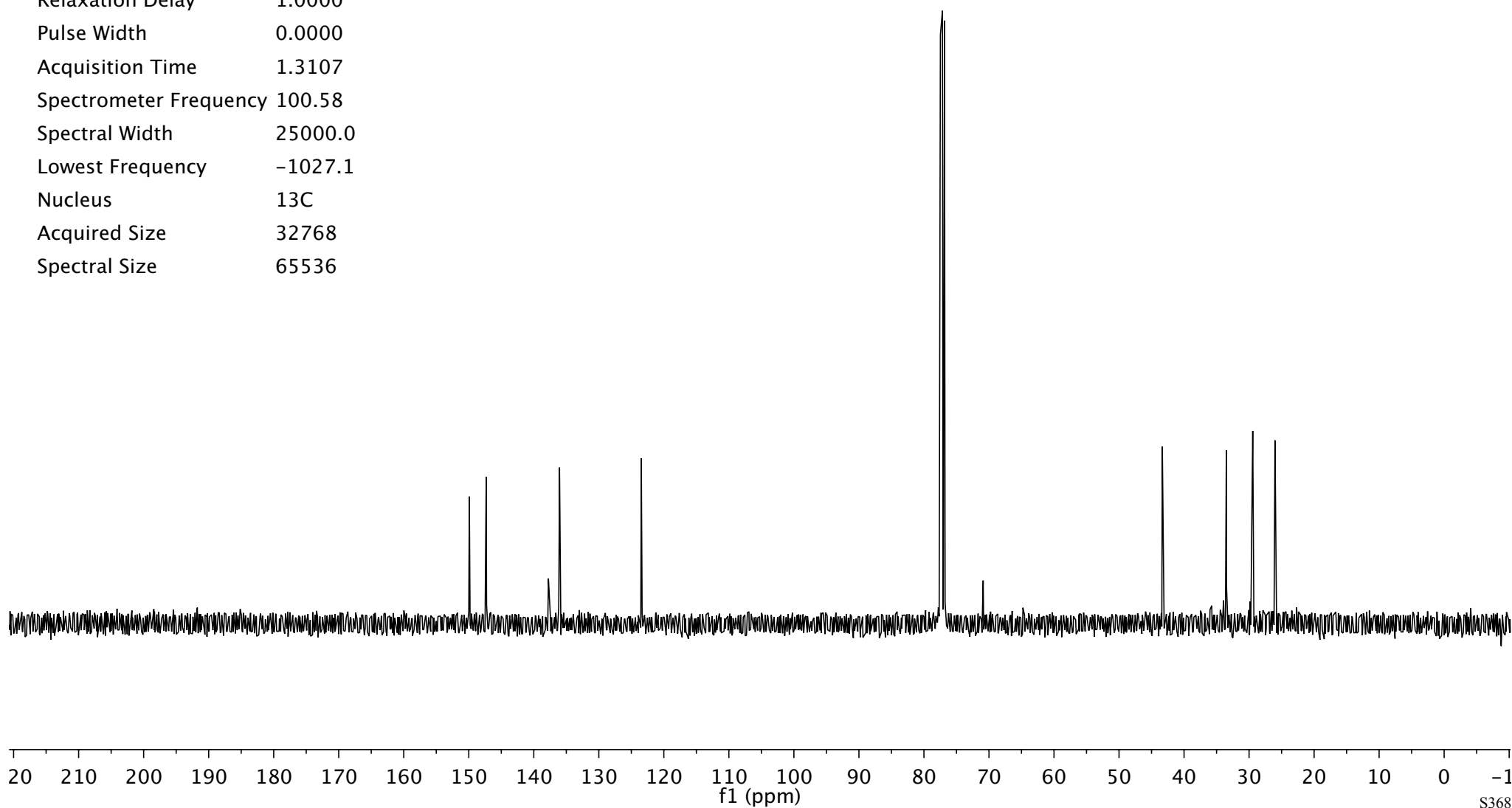
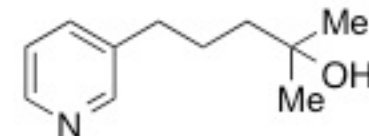


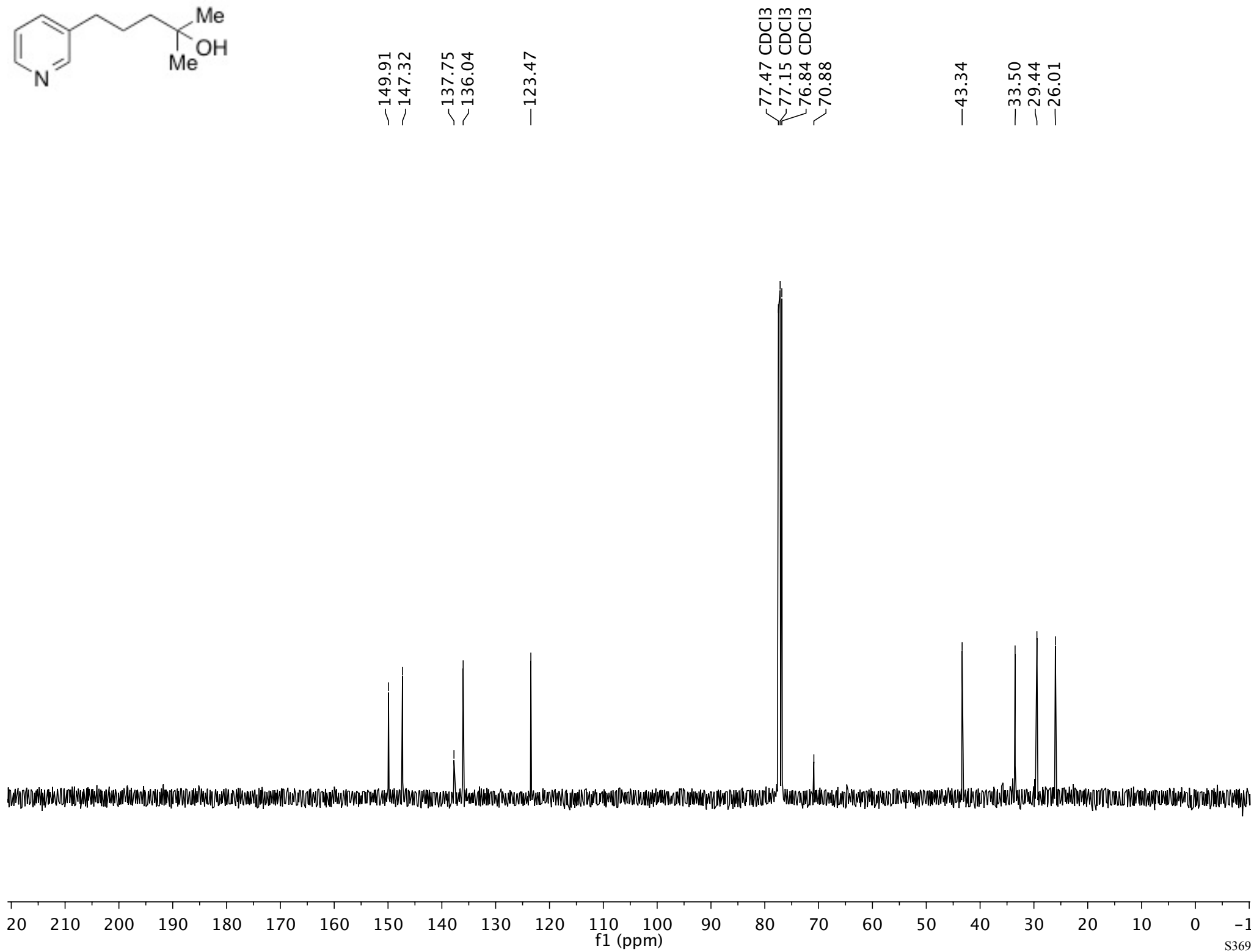
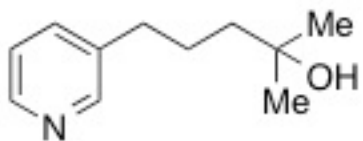
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	22
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1520.9
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



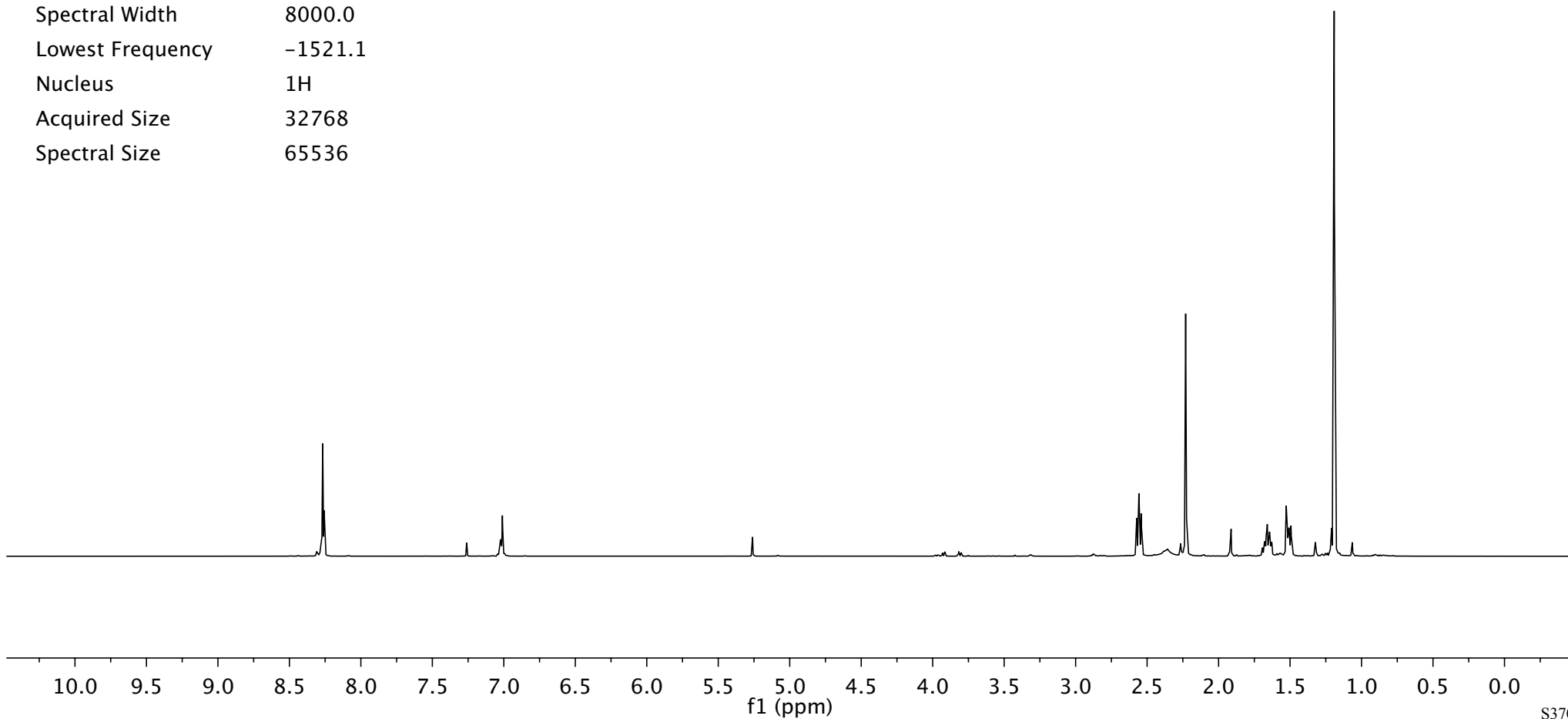
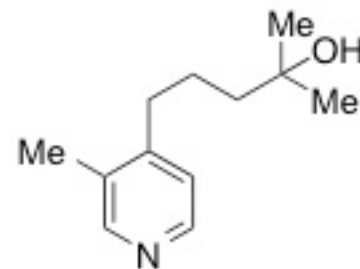


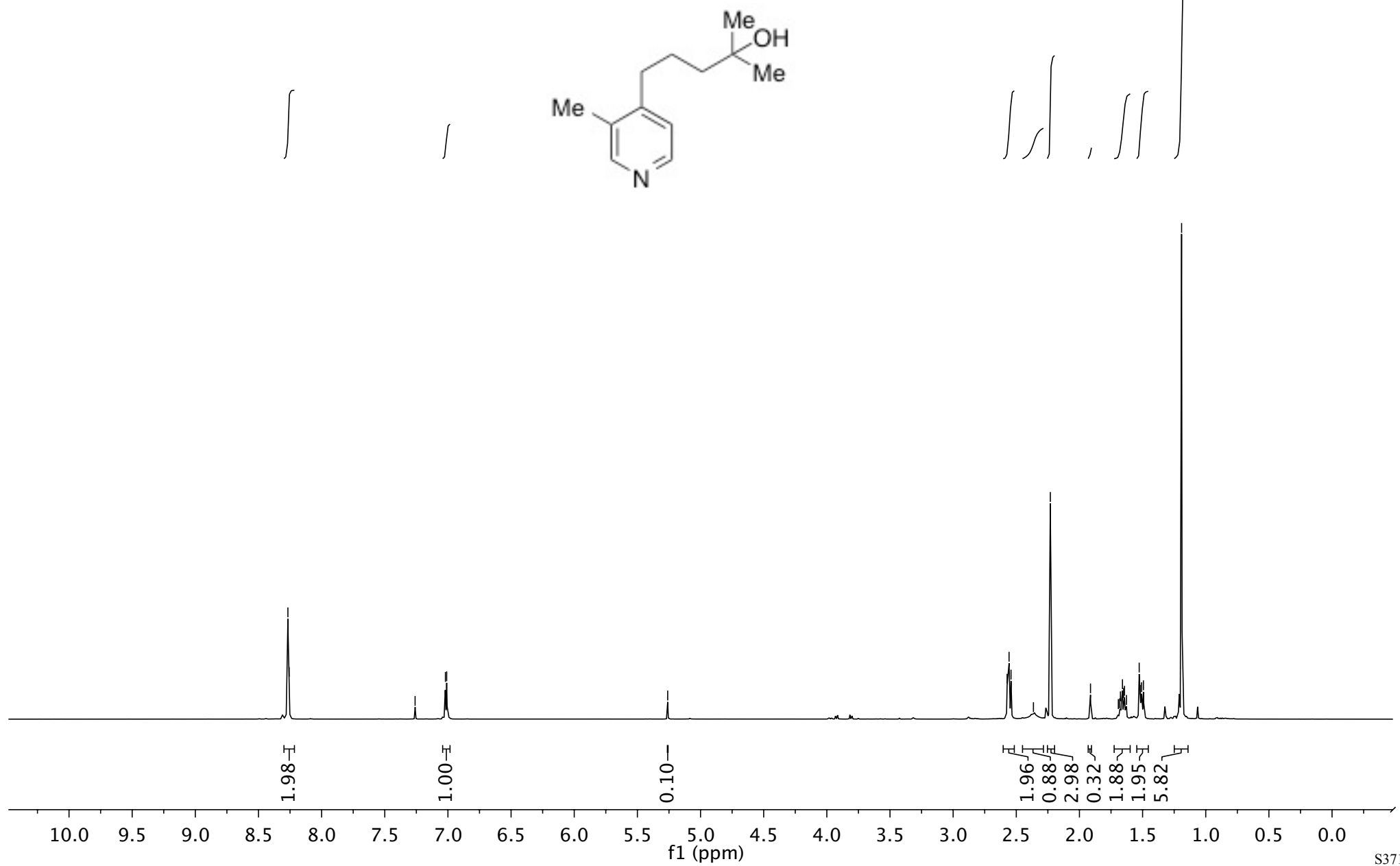
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3107
Spectrometer Frequency	100.58
Spectral Width	25000.0
Lowest Frequency	-1027.1
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



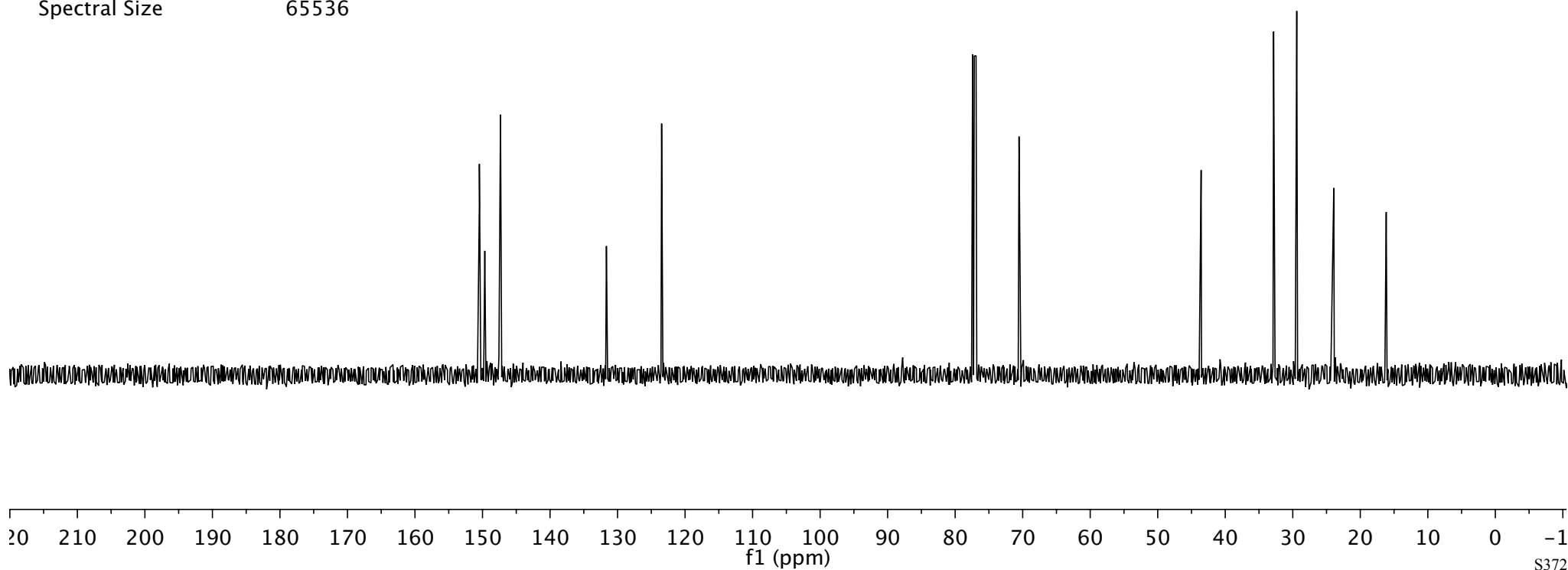
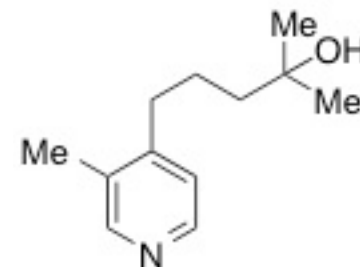


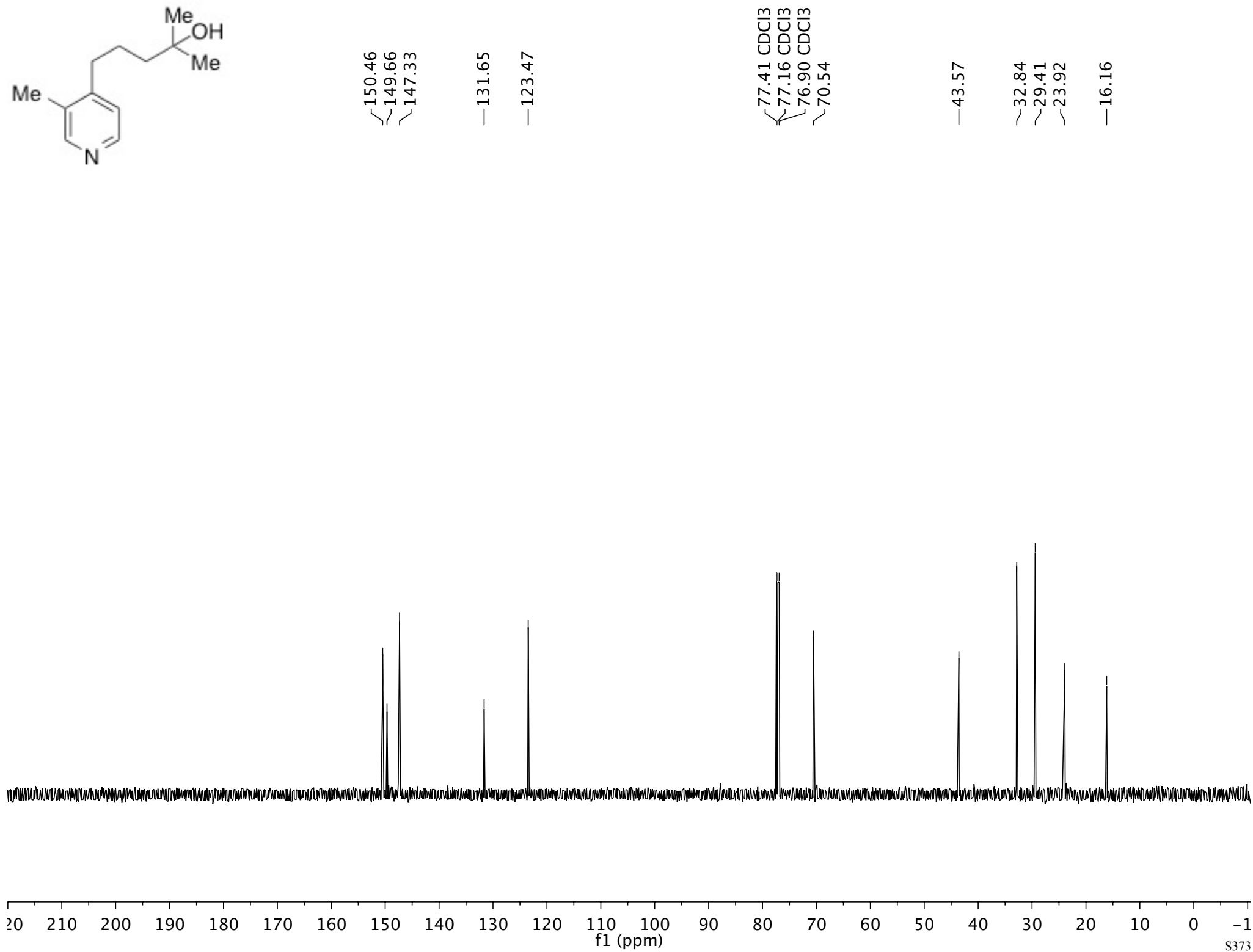
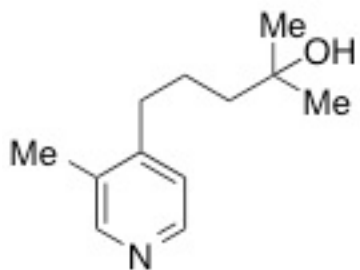
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	28
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



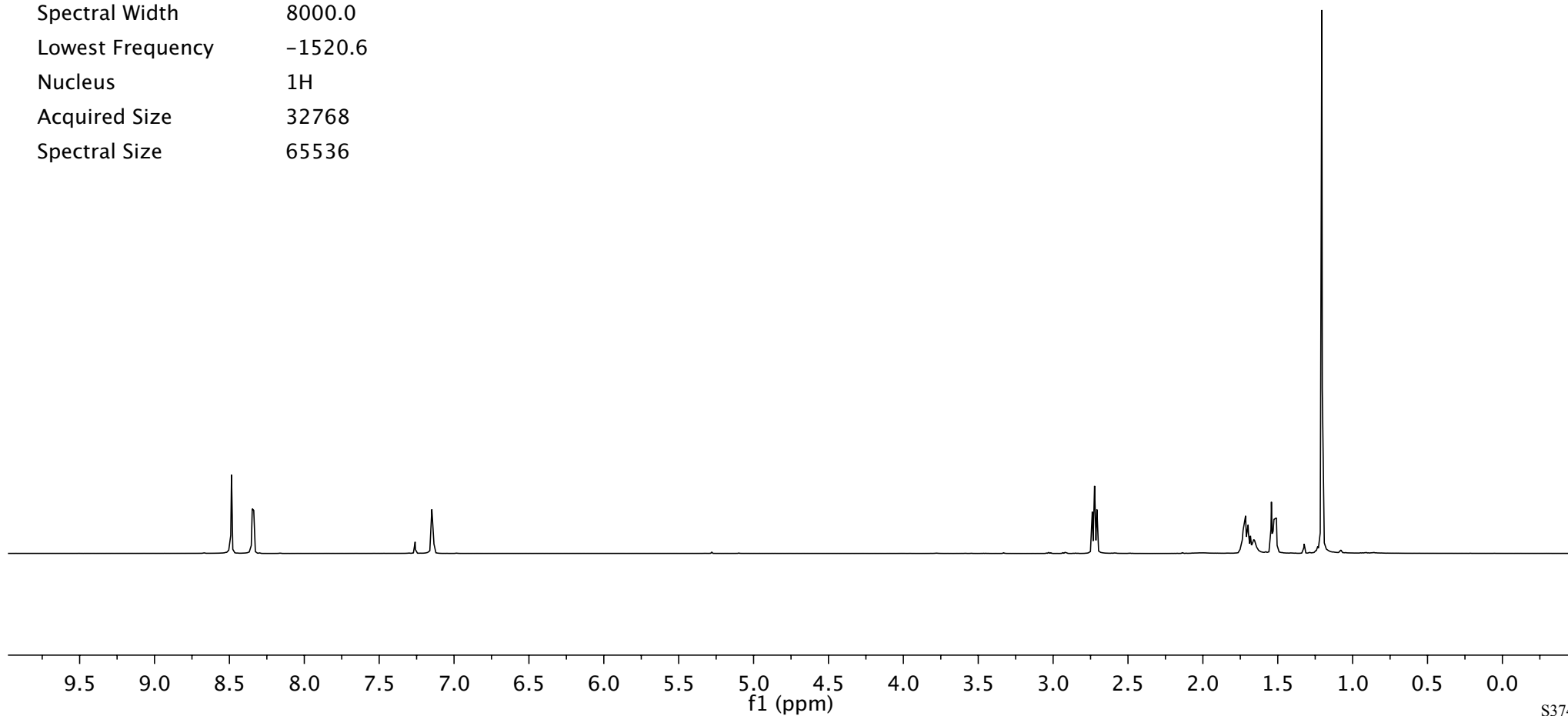
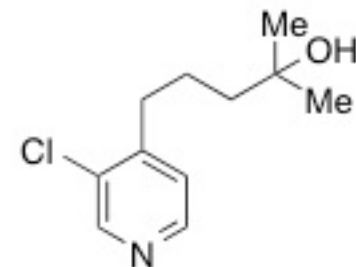


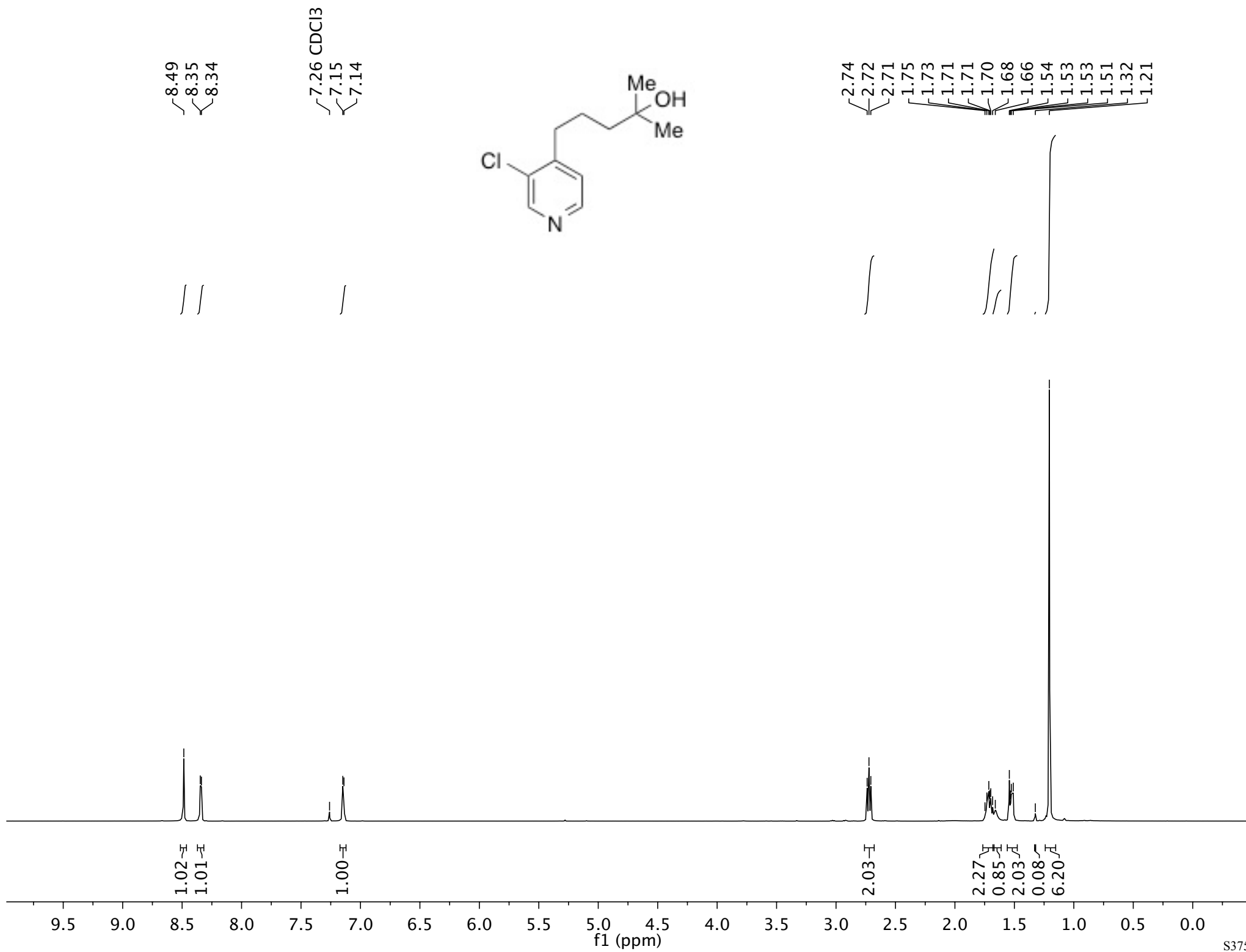
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2208.3
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



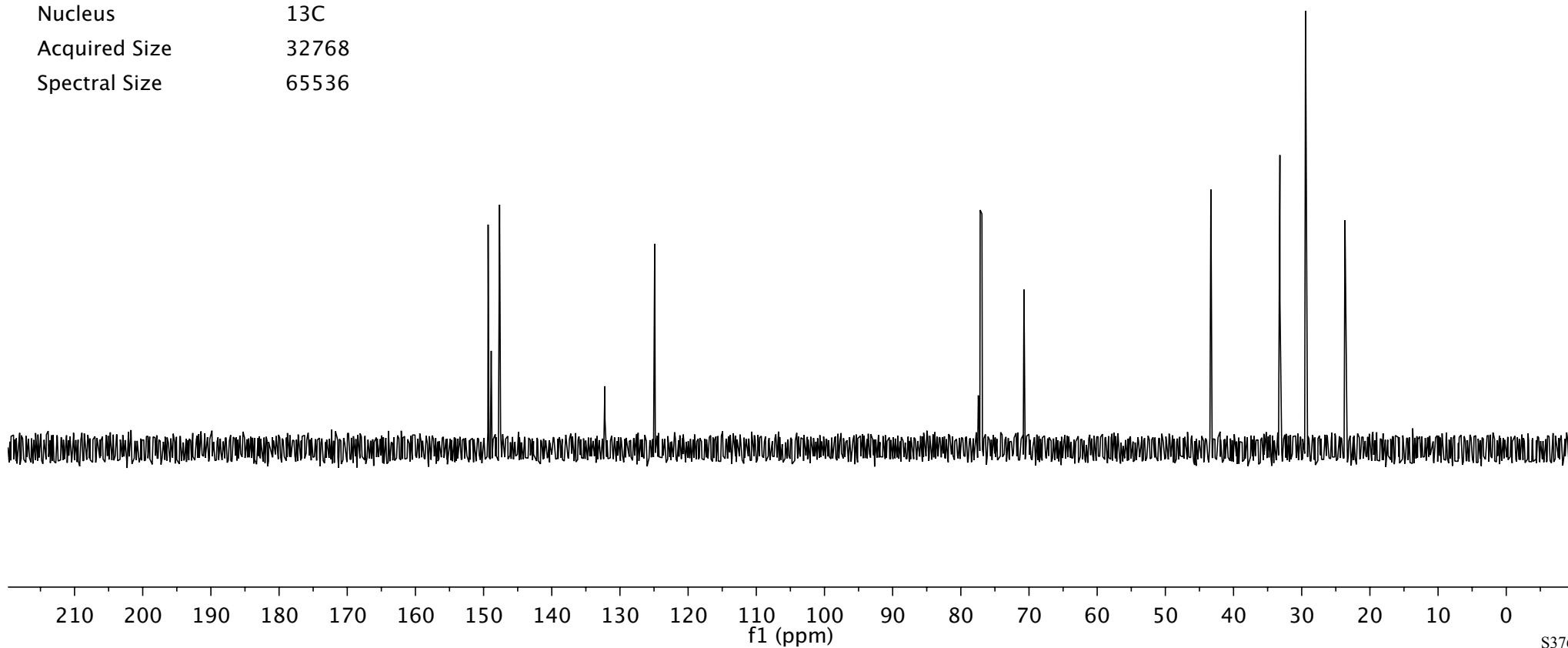
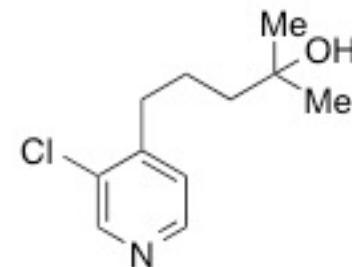


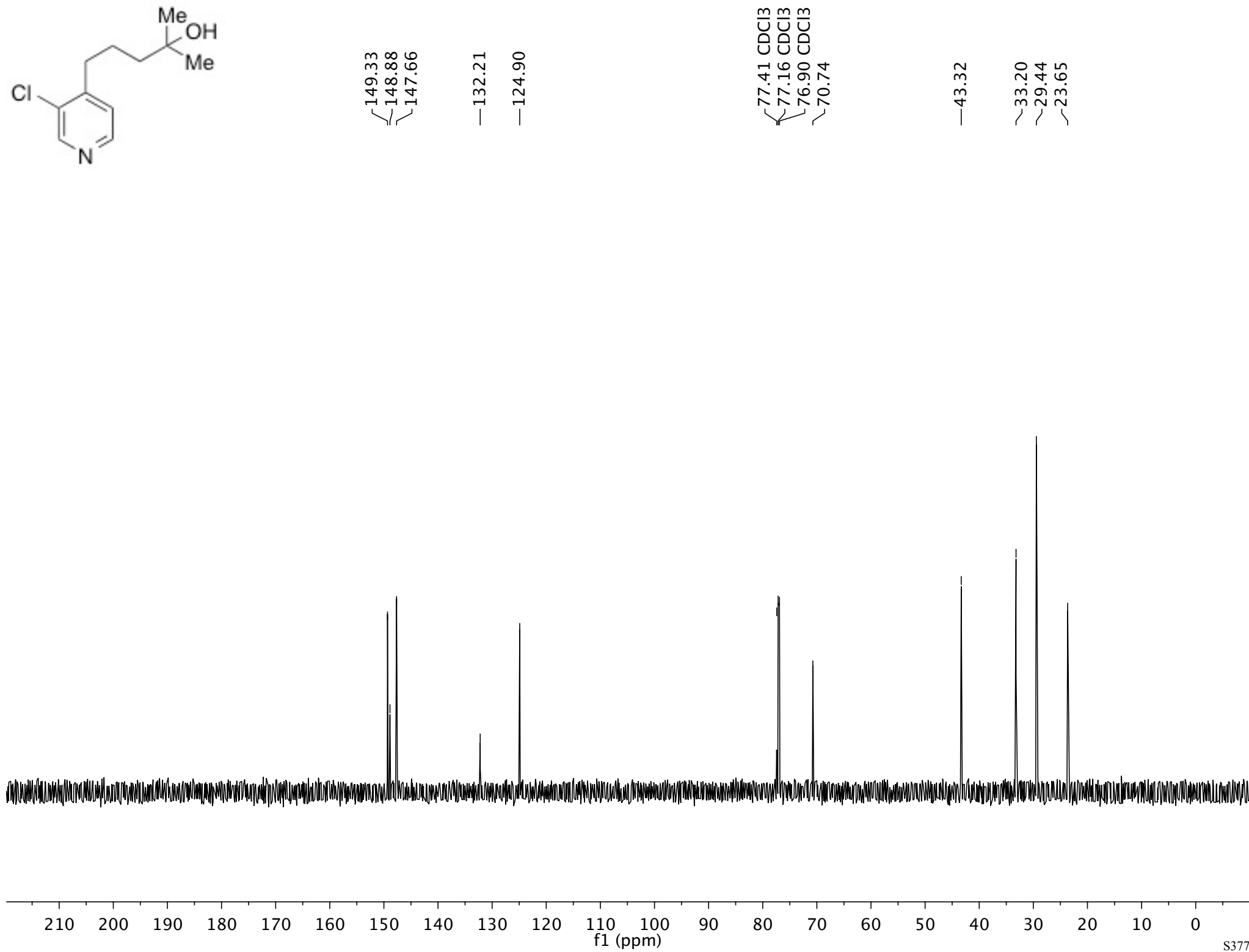
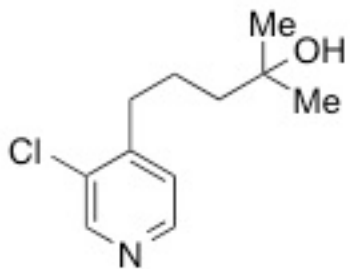
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	26
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1520.6
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

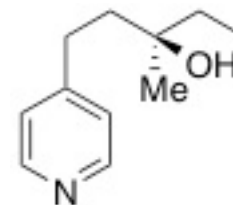




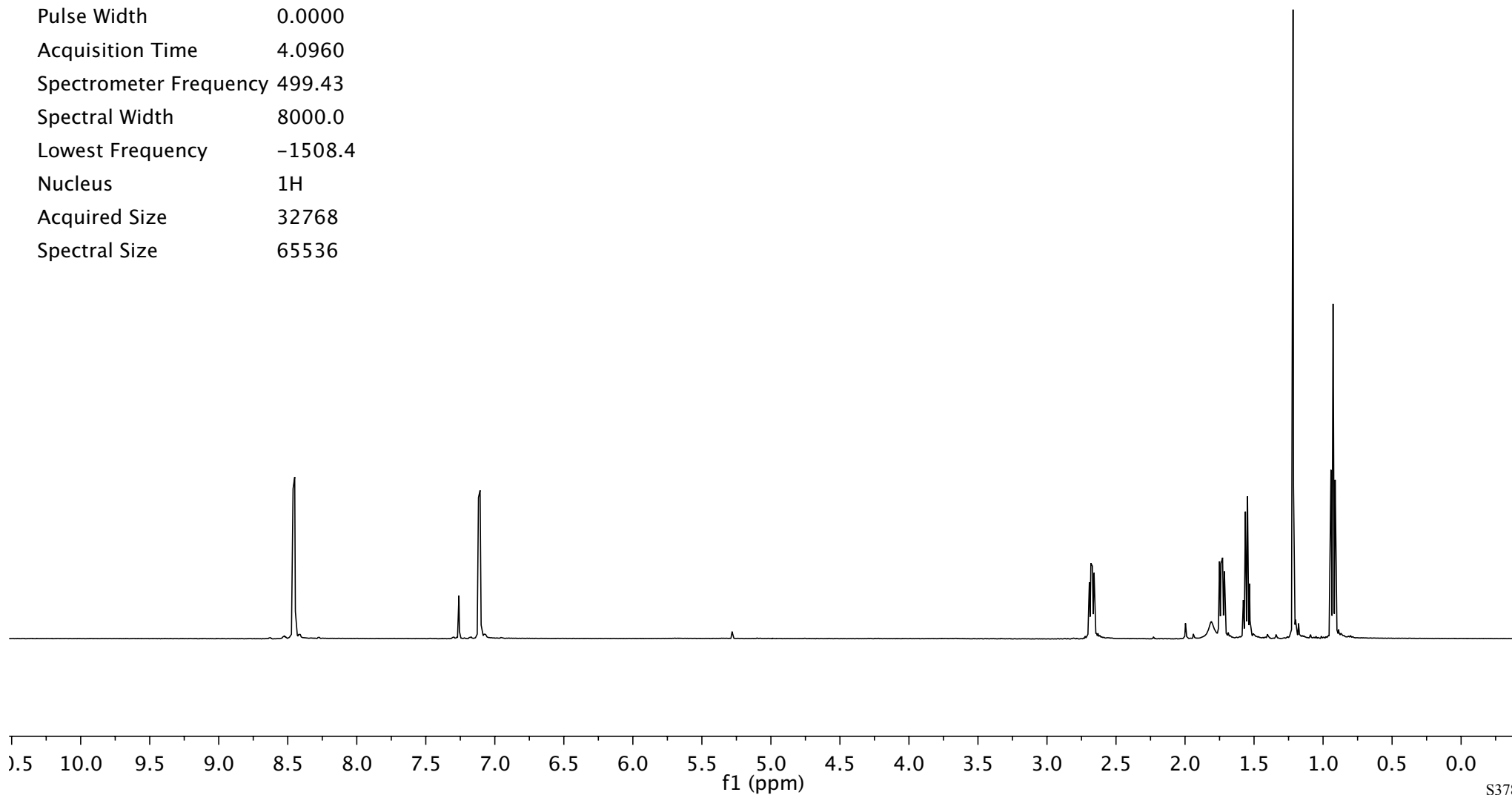
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2205.0
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

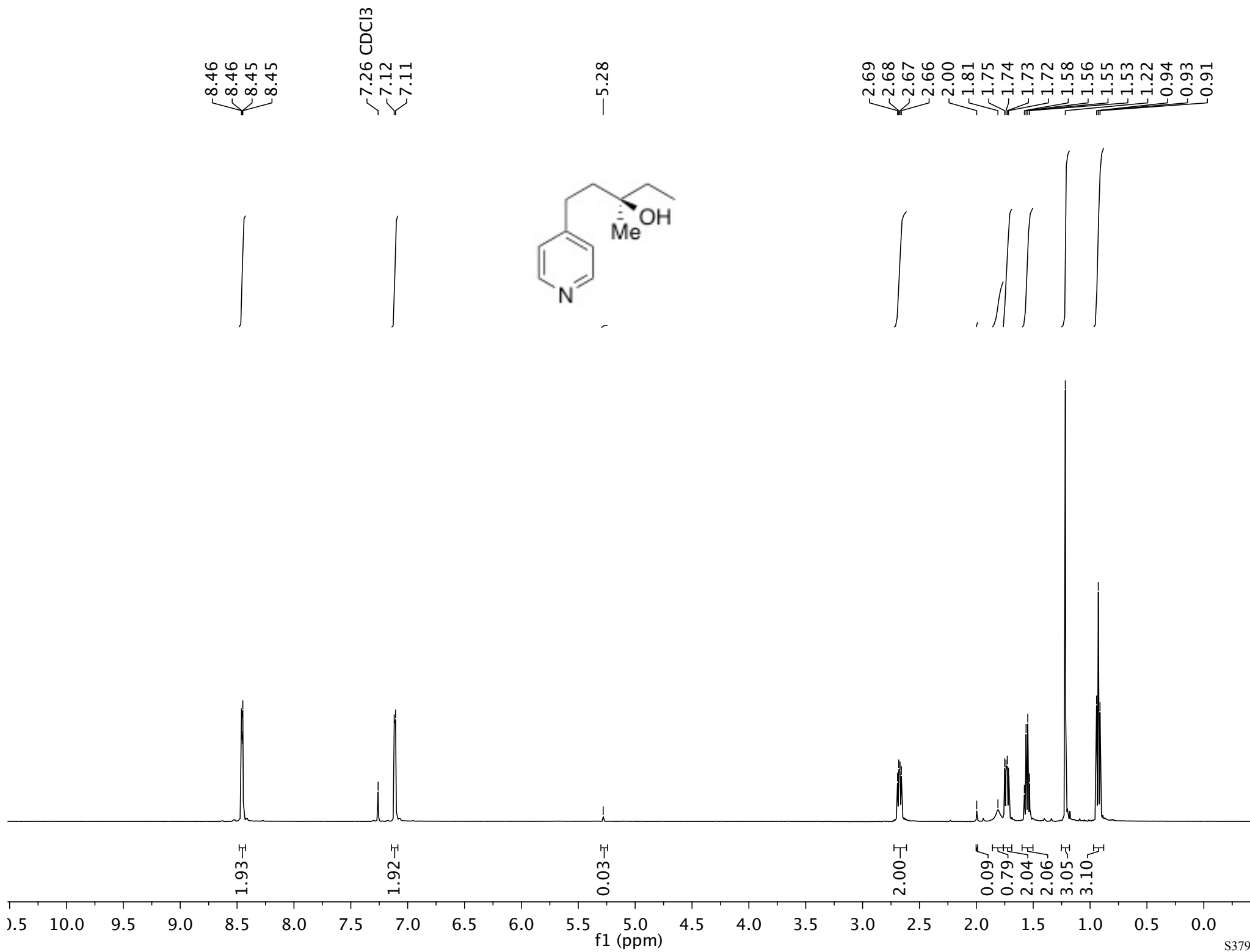




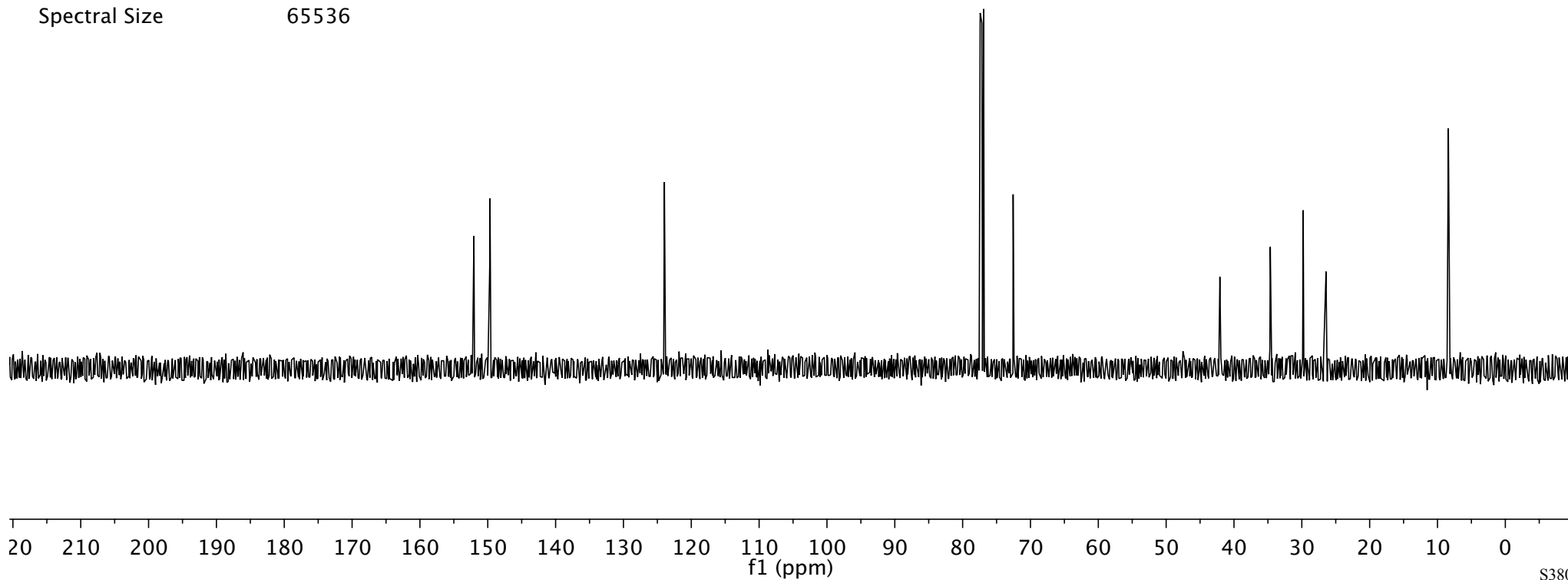
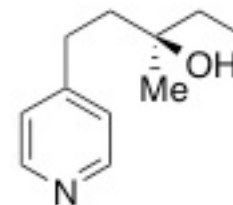


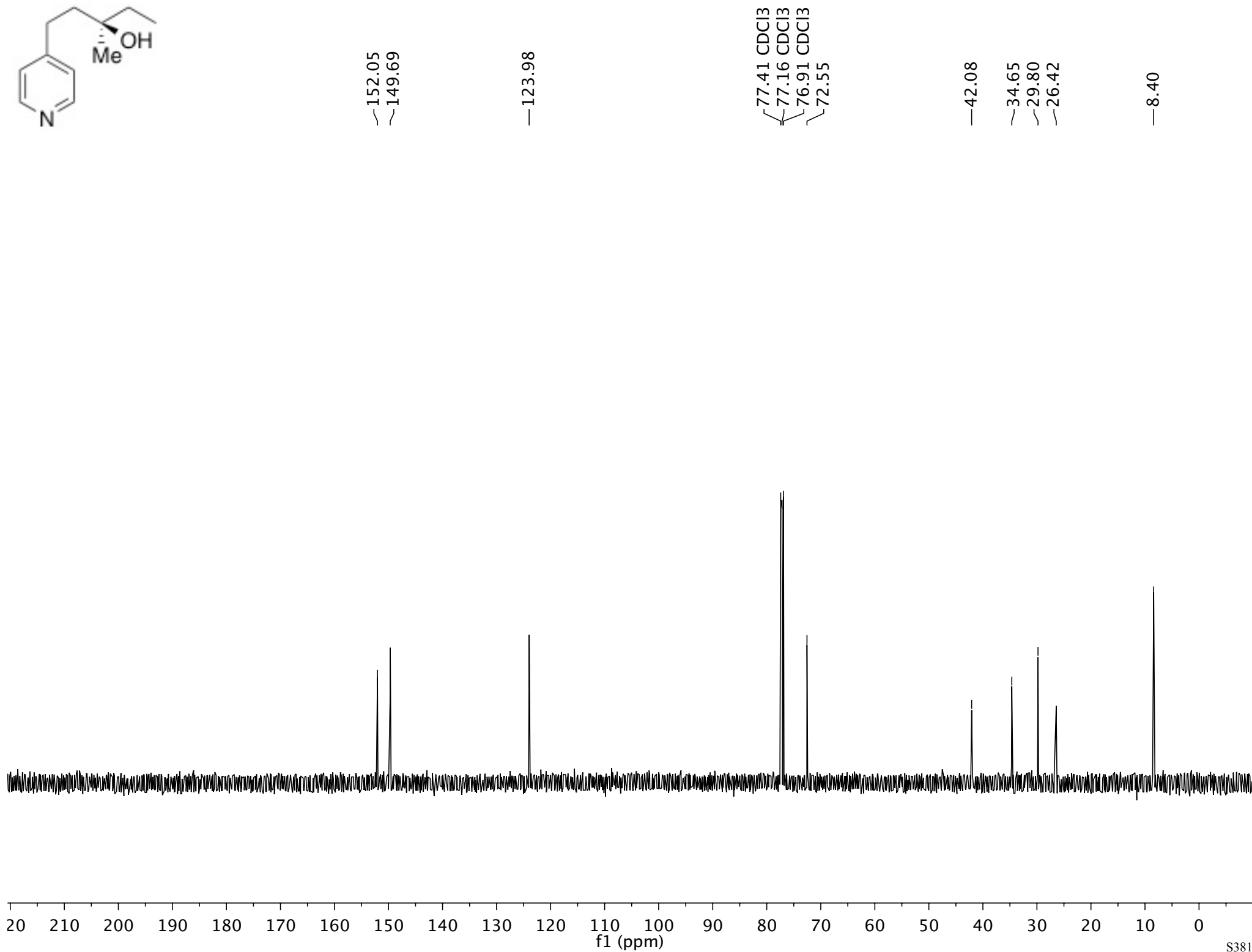
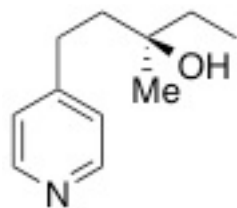
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	56
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	499.43
Spectral Width	8000.0
Lowest Frequency	-1508.4
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



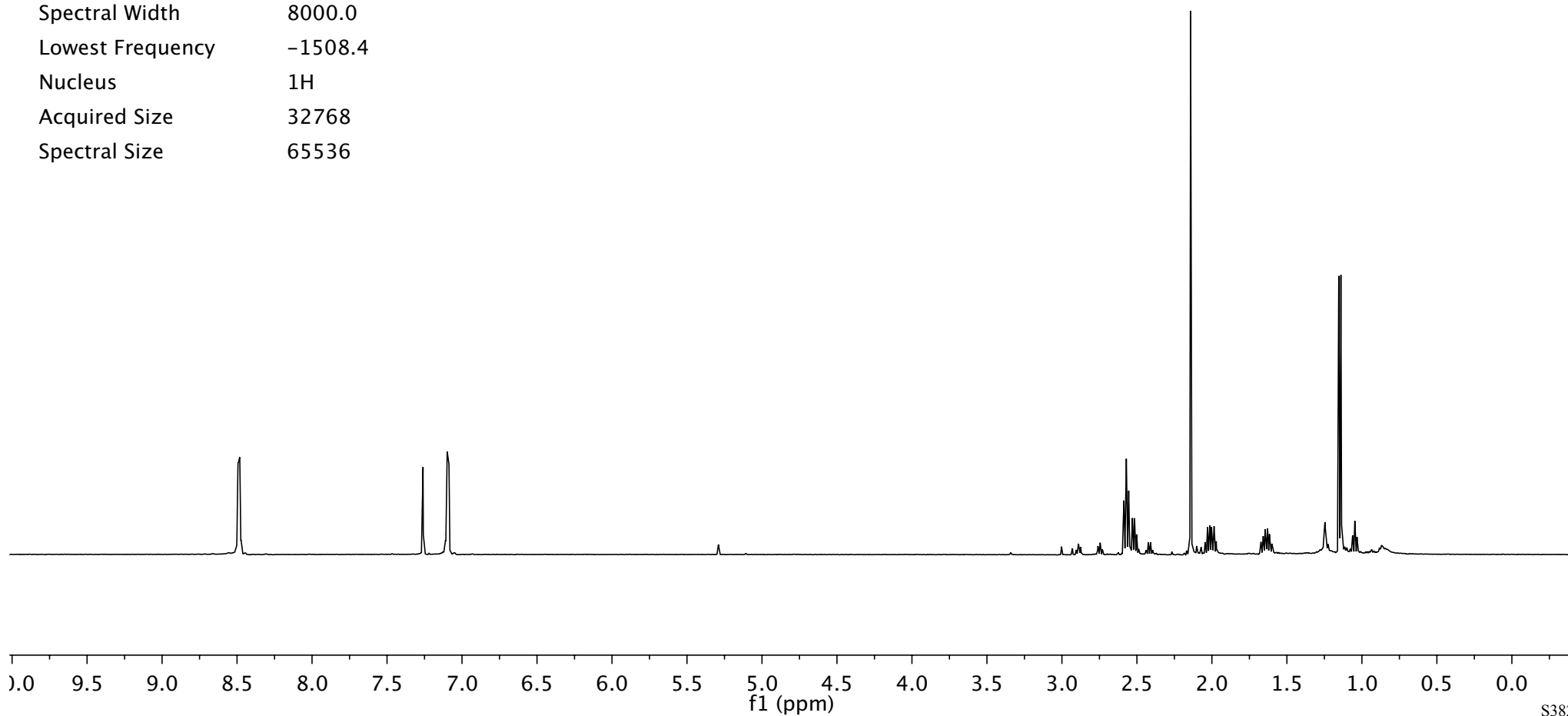
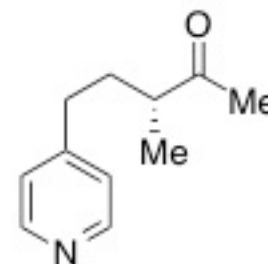


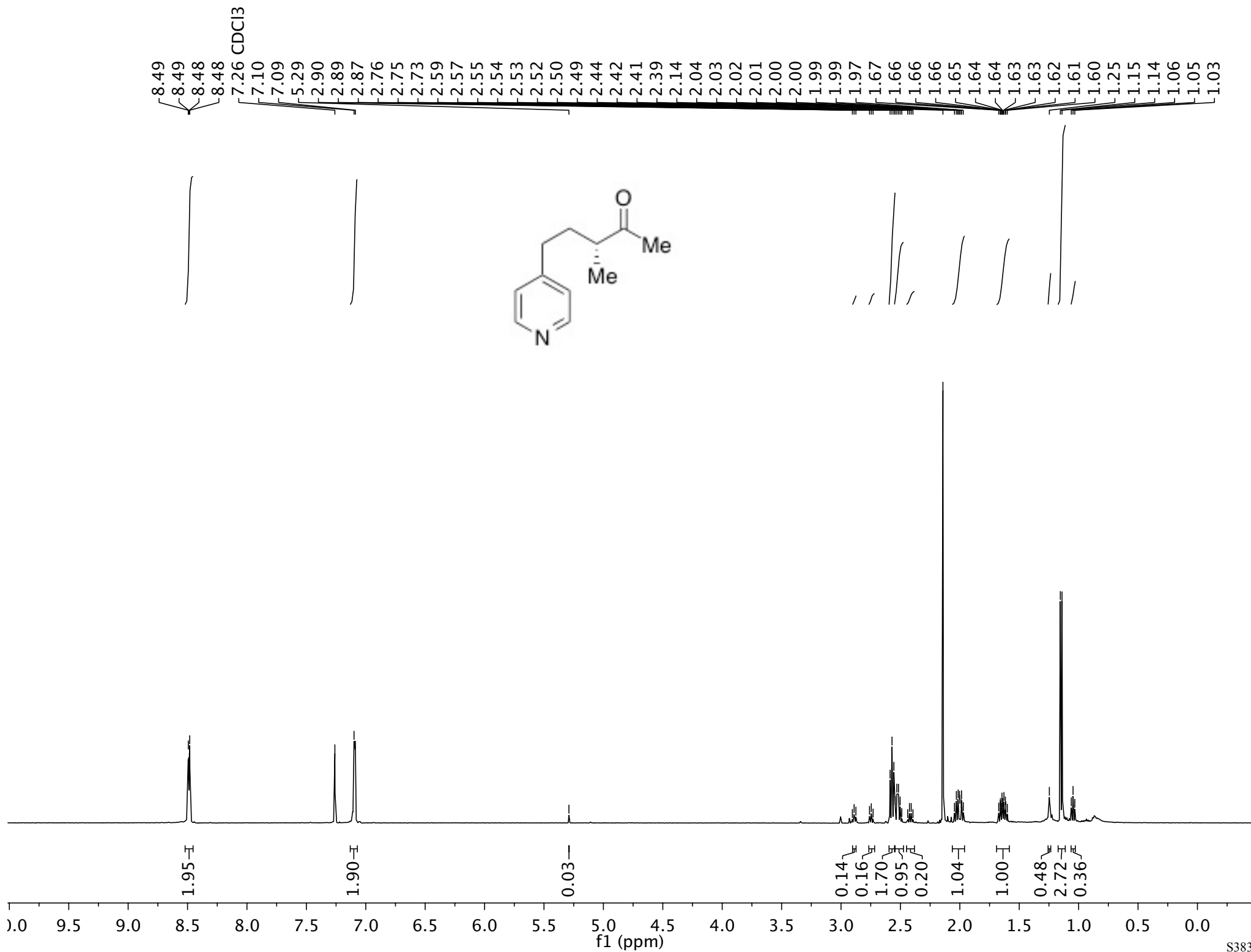
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2202.4
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



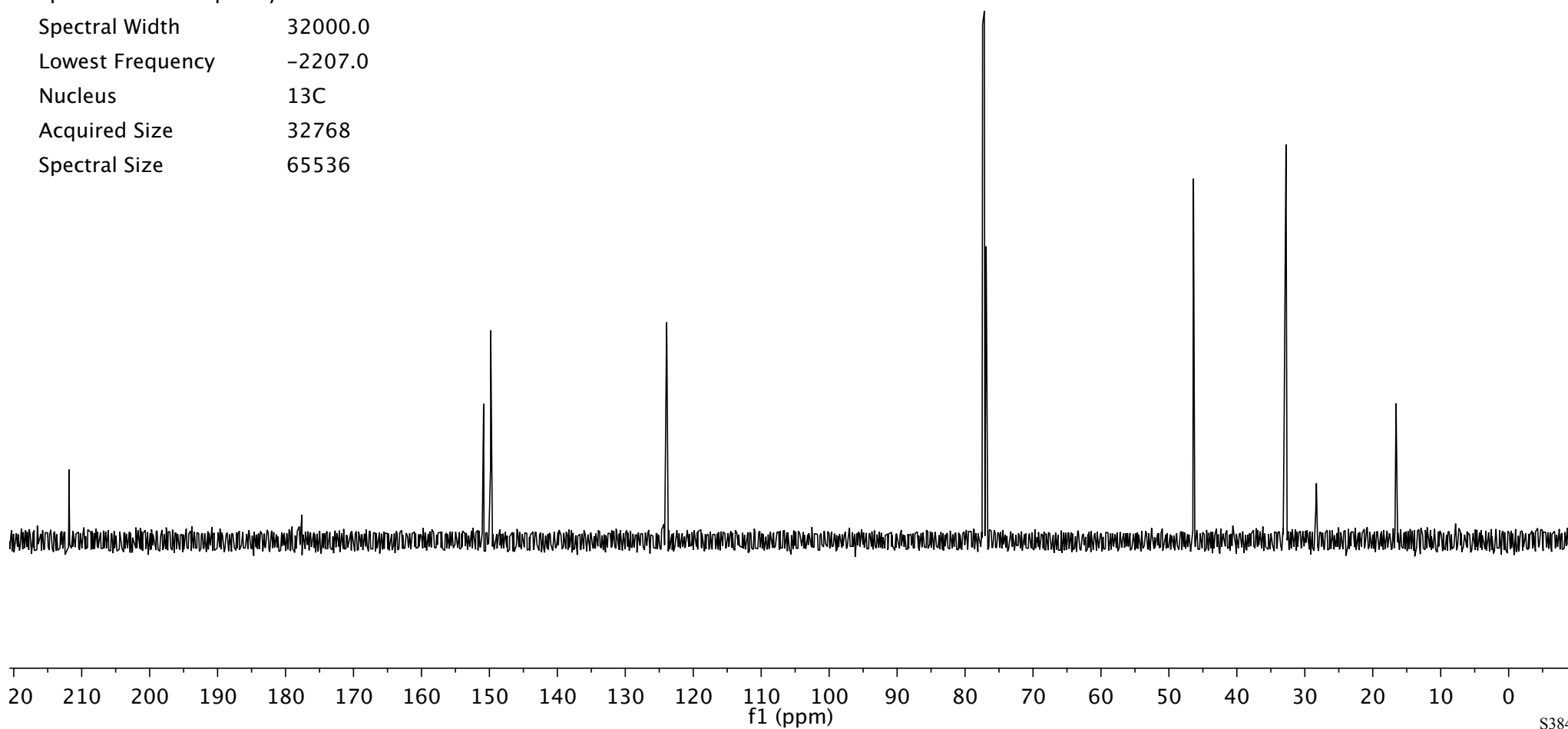
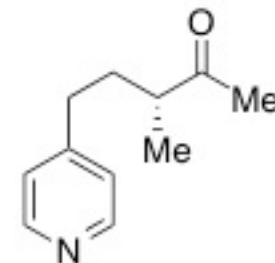


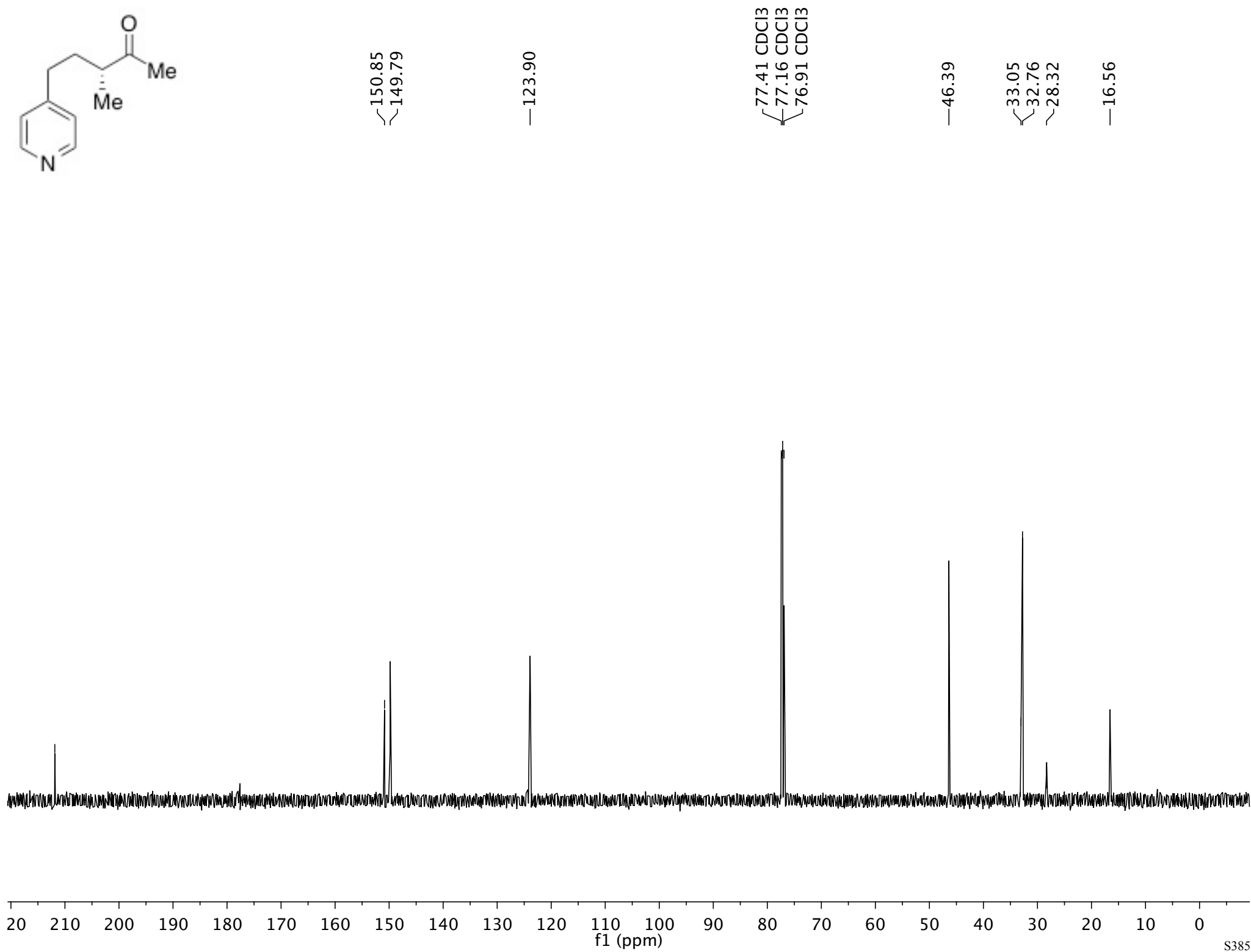
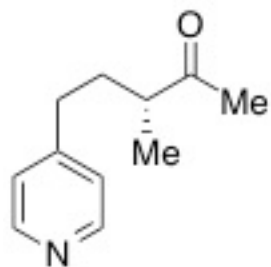
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	56
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	499.43
Spectral Width	8000.0
Lowest Frequency	-1508.4
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

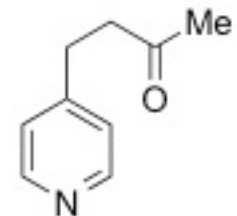




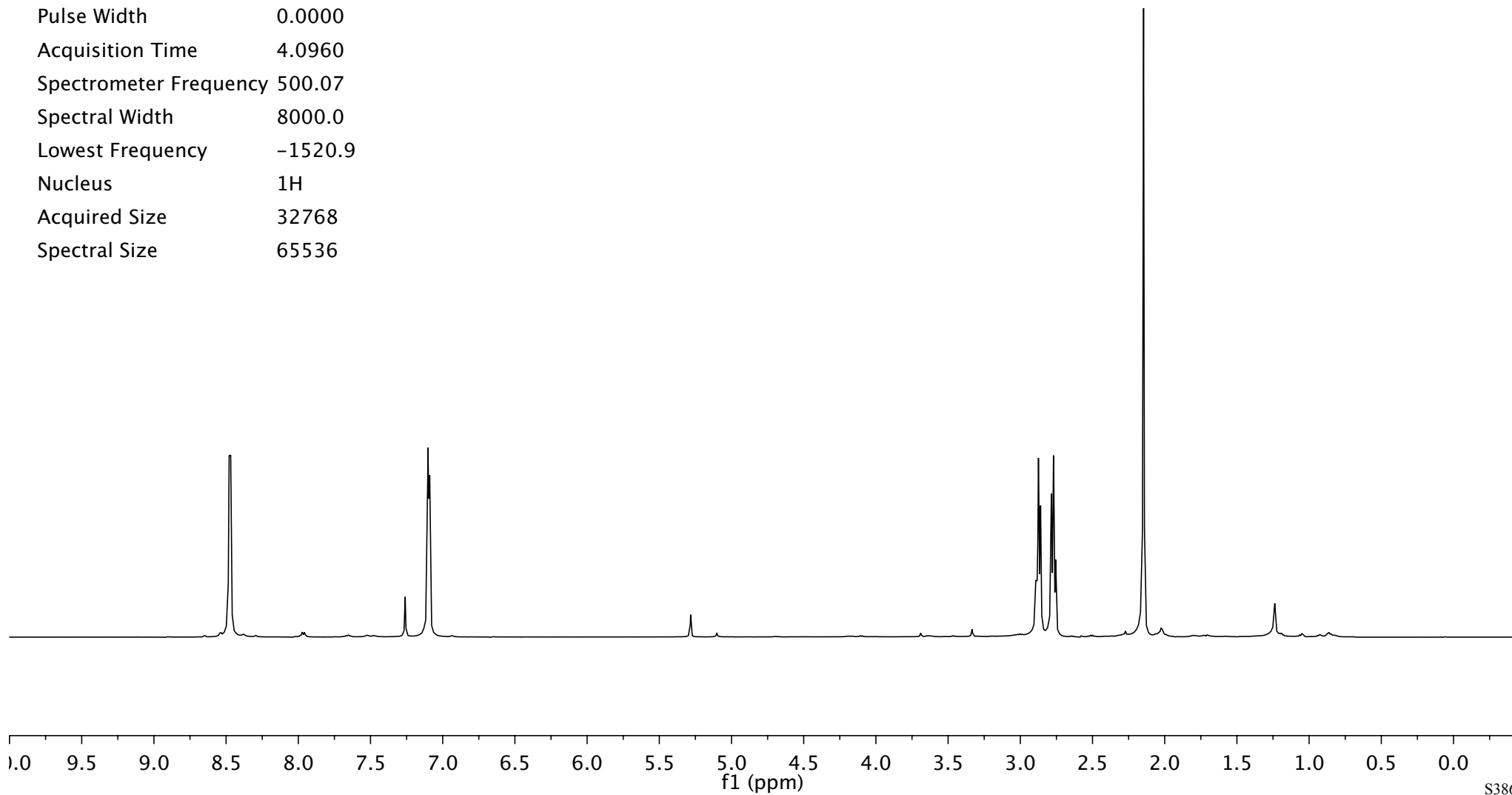
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2207.0
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

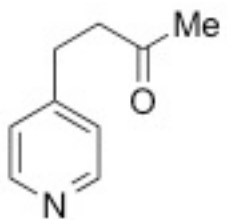






Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	32
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1520.9
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536





8.48
8.47

7.97
7.96

7.26 CDCl₃

7.10
7.09

5.28

2.89

2.87

2.86

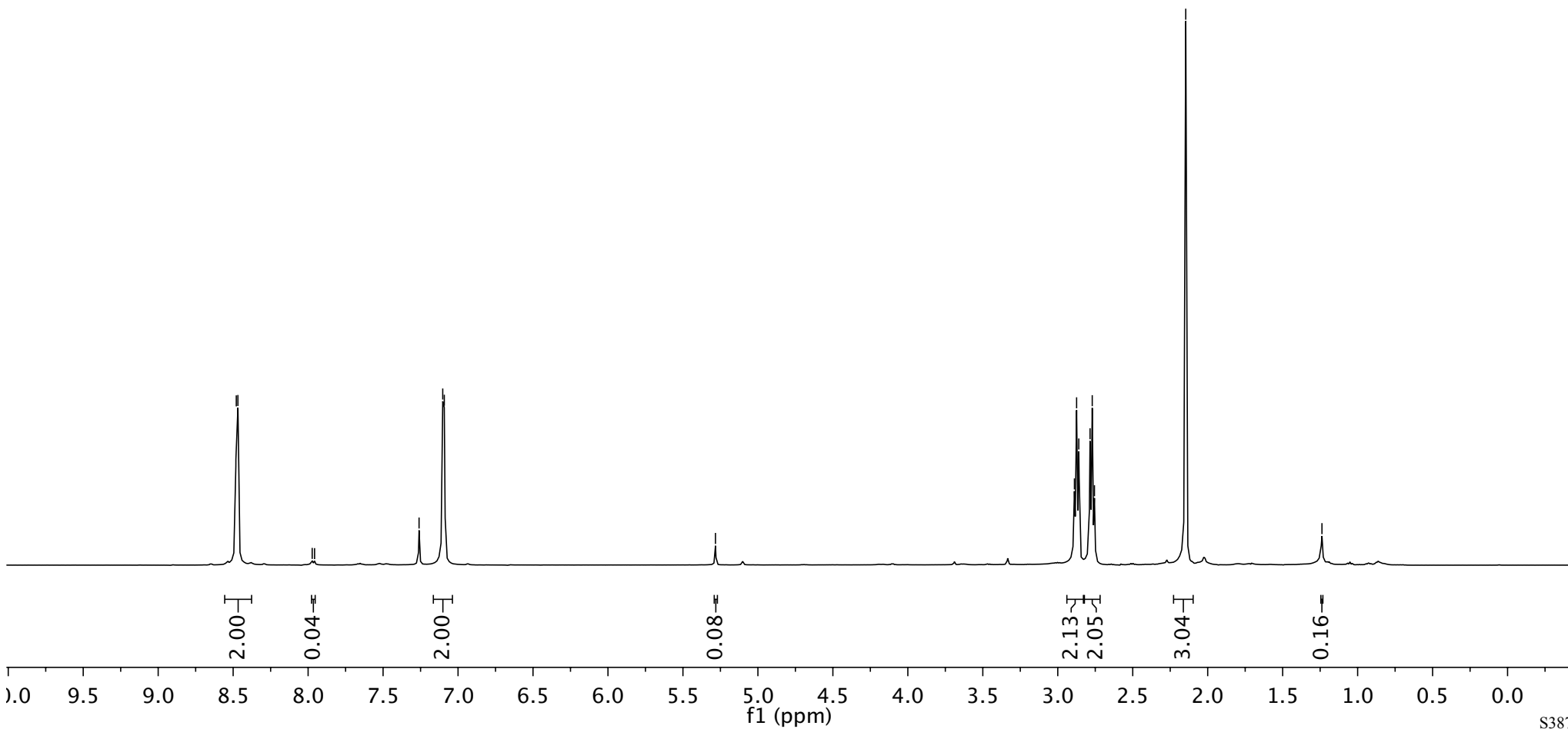
2.78

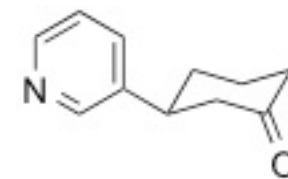
2.77

2.76

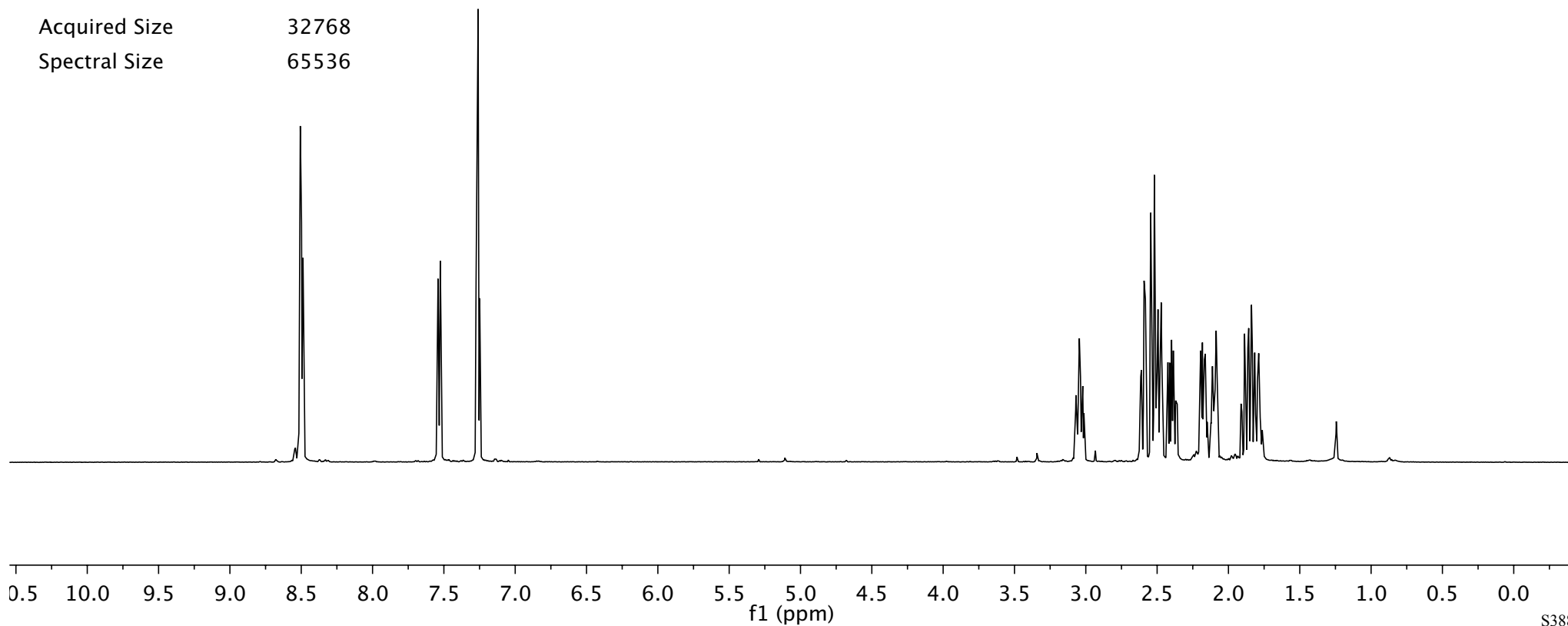
2.15

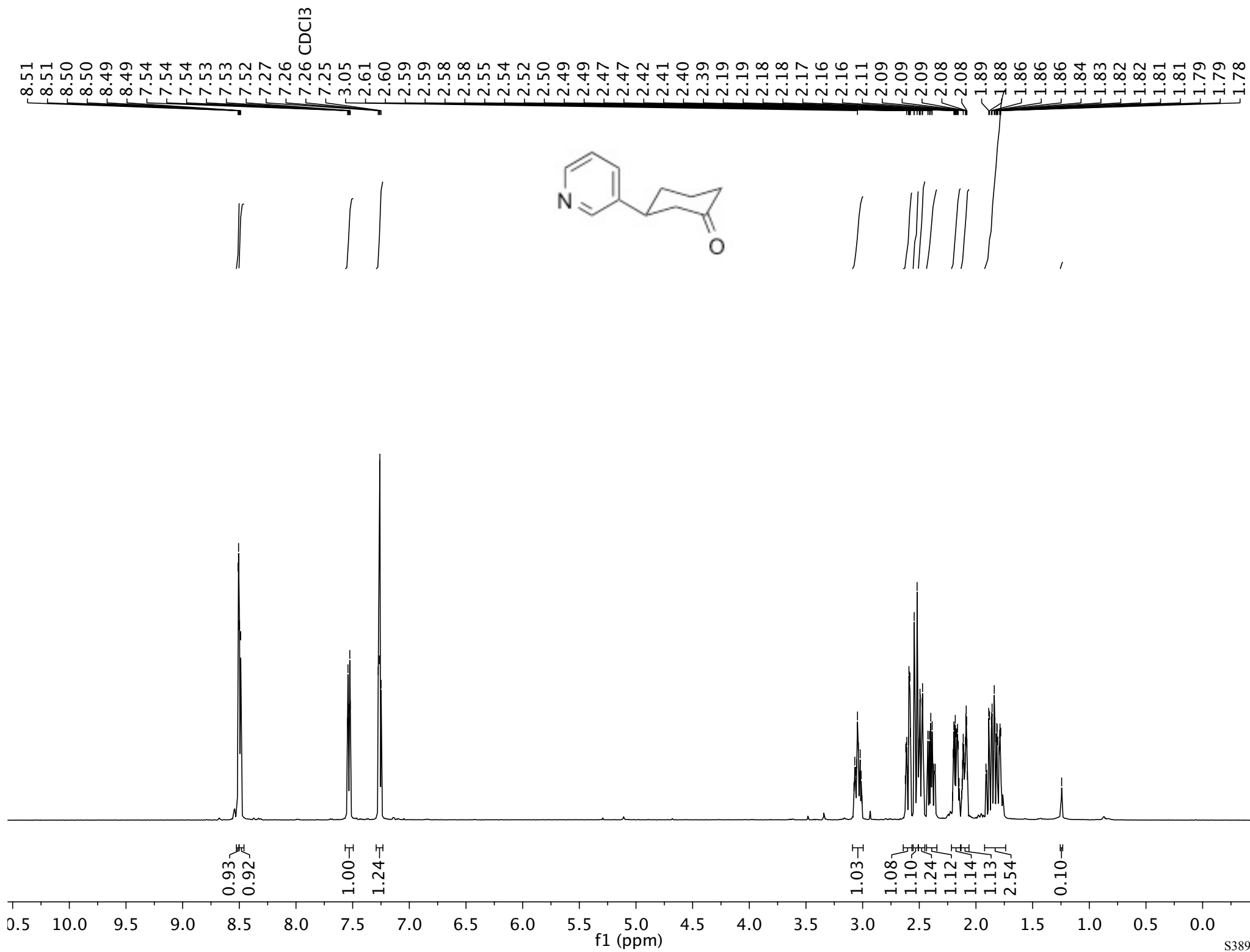
1.24

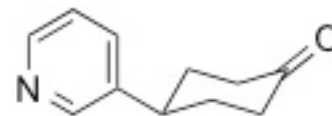




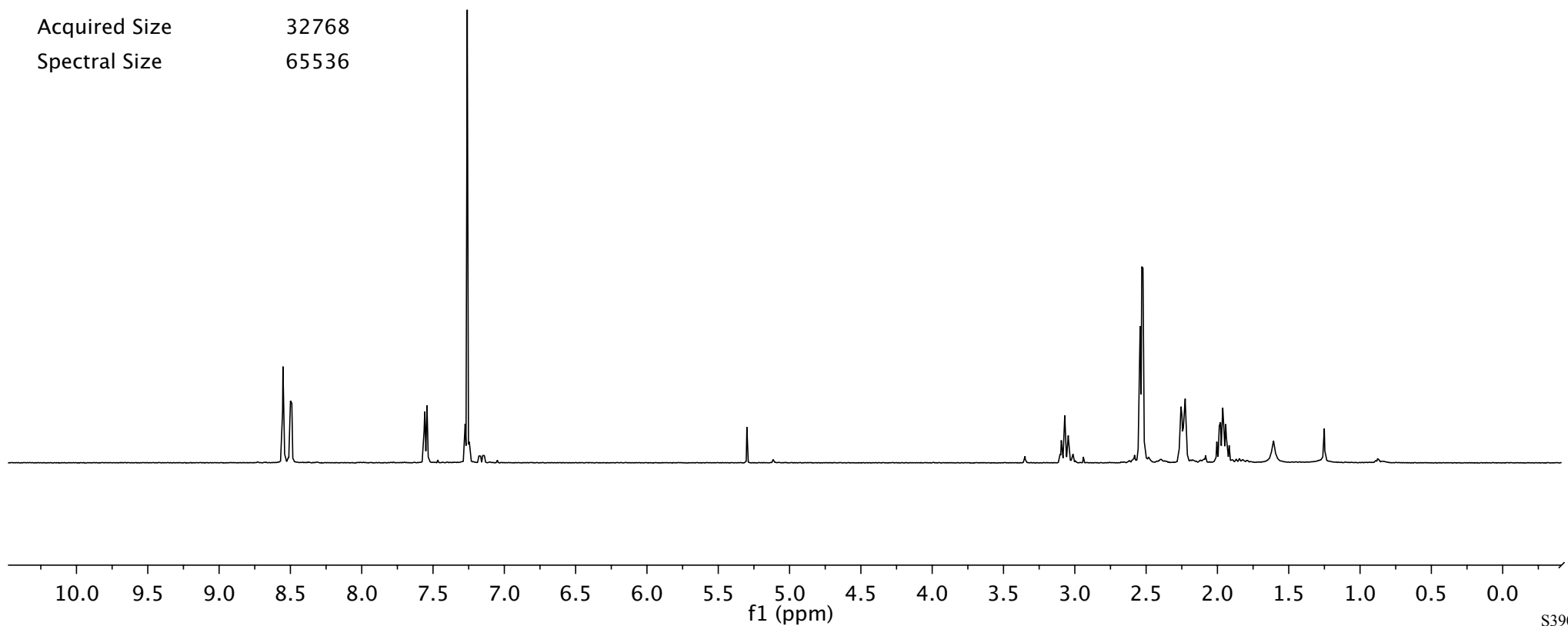
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	48
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1520.9
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

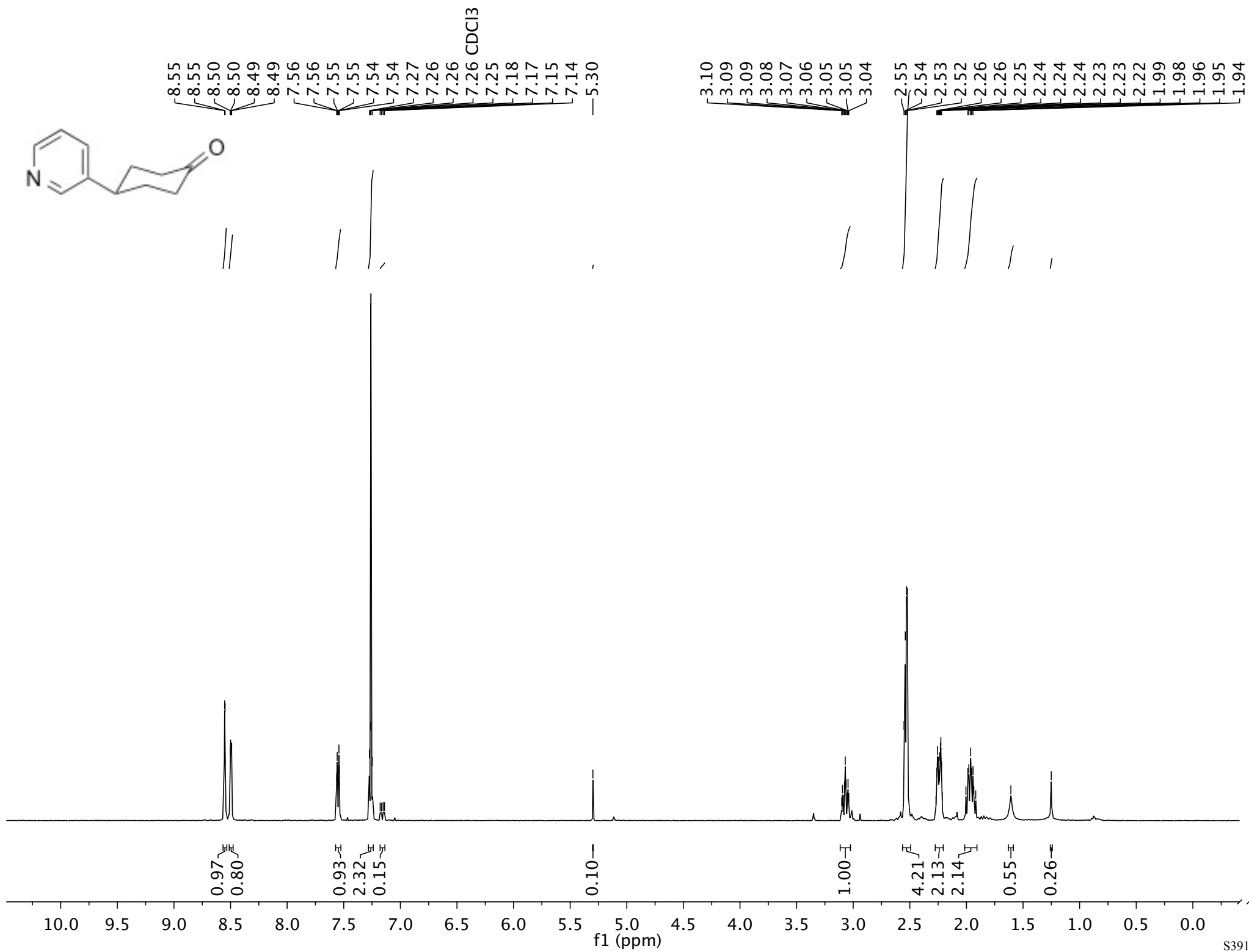




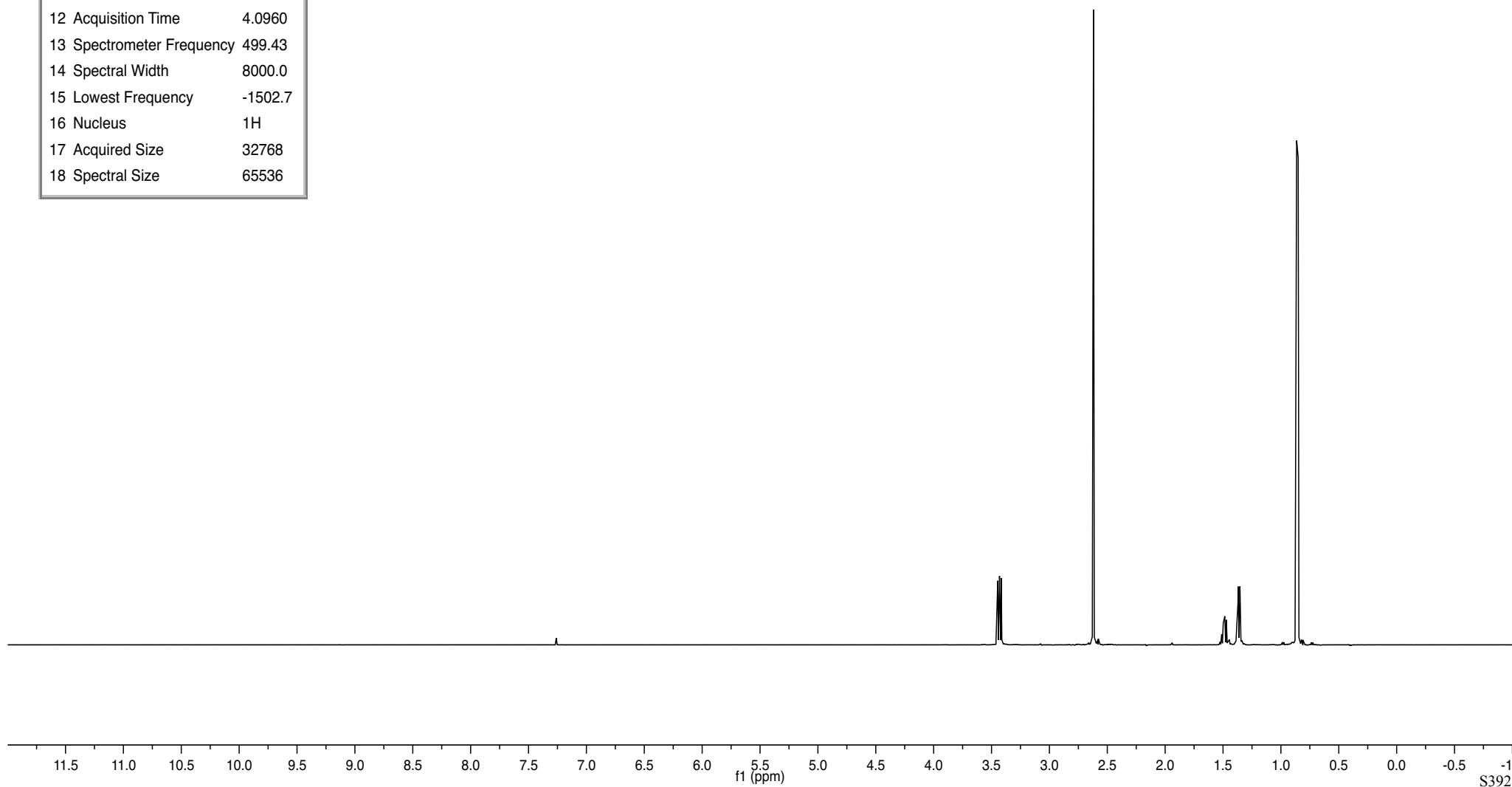
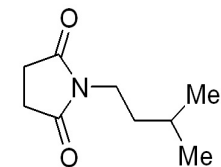


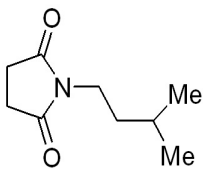
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1520.6
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536





	Parameter	Value
1	Origin	Varian
2	Spectrometer	inova
3	Solvent	CDCl3
4	Temperature	20.0
5	Pulse Sequence	s2pul
6	Experiment	1D
7	Probe	QUADG
8	Number of Scans	8
9	Receiver Gain	44
10	Relaxation Delay	0.0000
11	Pulse Width	0.0000
12	Acquisition Time	4.0960
13	Spectrometer Frequency	499.43
14	Spectral Width	8000.0
15	Lowest Frequency	-1502.7
16	Nucleus	¹ H
17	Acquired Size	32768
18	Spectral Size	65536

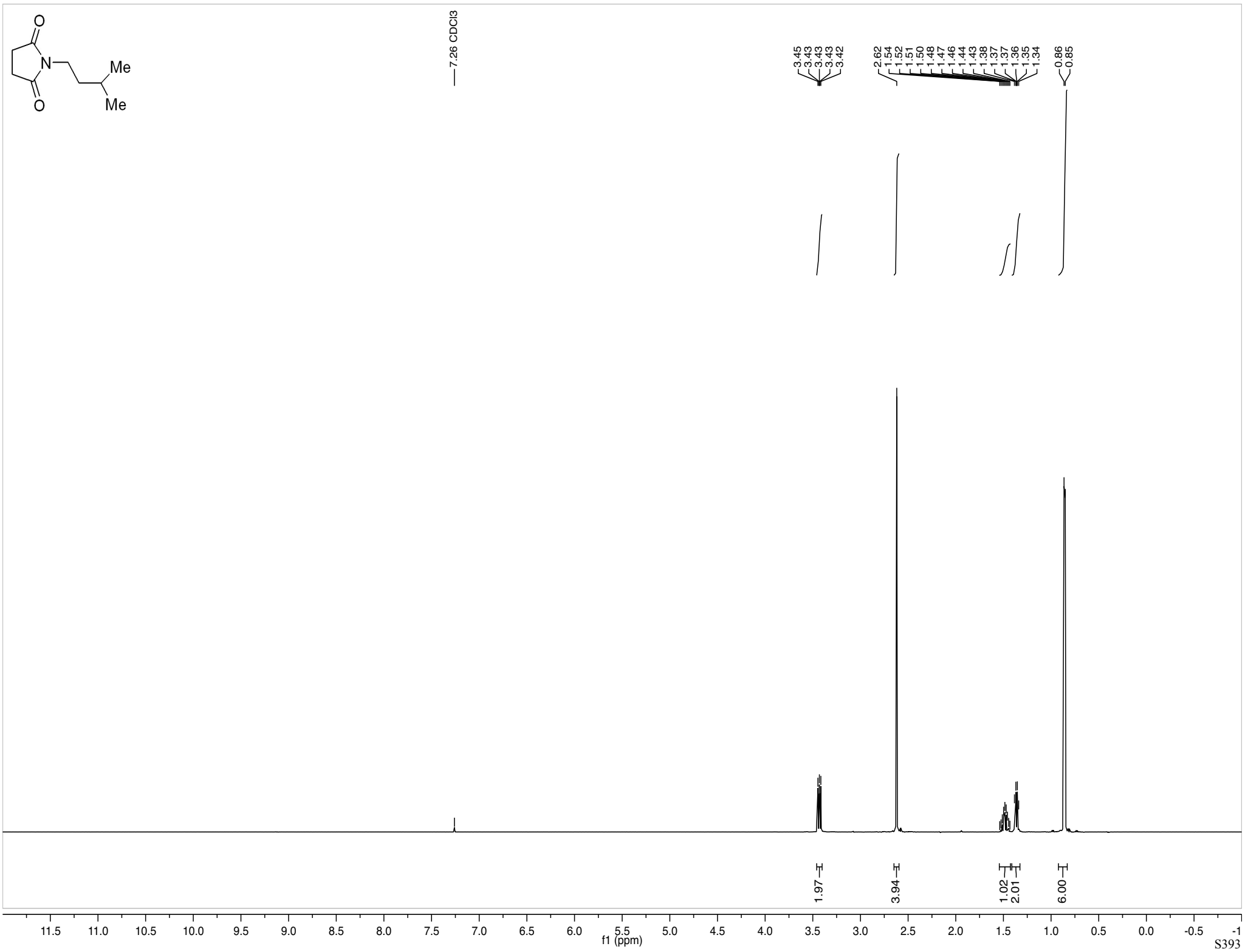




— 7.26 CDCl₃

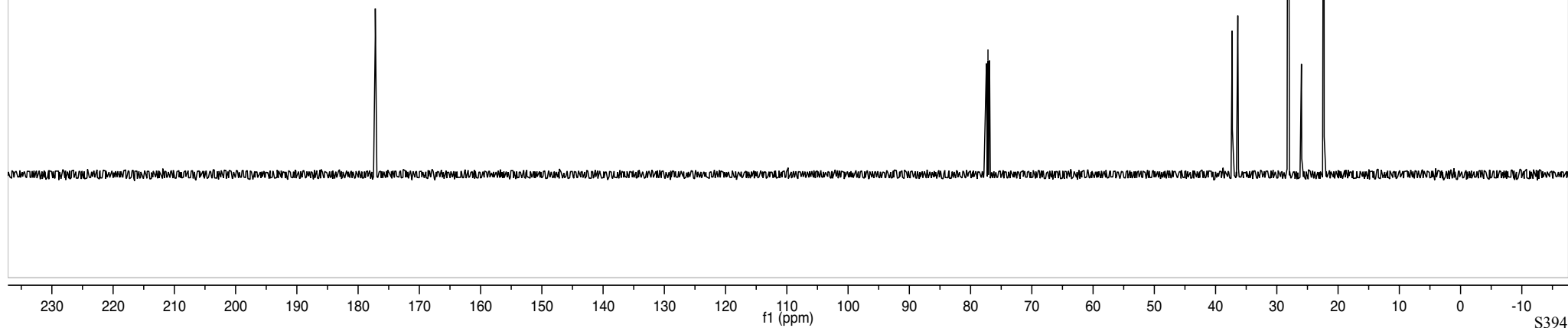
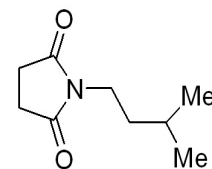
3.45
3.43
3.43
3.42
2.62
1.54
1.52
1.51
1.50
1.48
1.47
1.46
1.44
1.43
1.38
1.37
1.36
1.35
1.34
0.86
0.85

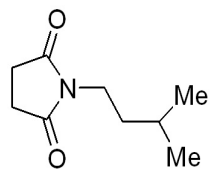
1.97
3.94
1.02
2.01
6.00



	Parameter	Value
1	Origin	Varian
2	Spectrometer	inova
3	Solvent	CDCl3
4	Temperature	20.0
5	Pulse Sequence	s2pul
6	Experiment	1D
7	Probe	QUADG
8	Number of Scans	48
9	Receiver Gain	60
10	Relaxation Delay	1.0000
11	Pulse Width	0.0000
12	Acquisition Time	1.0240
13	Spectrometer Frequency	125.60
14	Spectral Width	32000.0
15	Lowest Frequency	-2188.2
16	Nucleus	¹³ C
17	Acquired Size	32768
18	Spectral Size	65536

— 77.16 CDCl₃



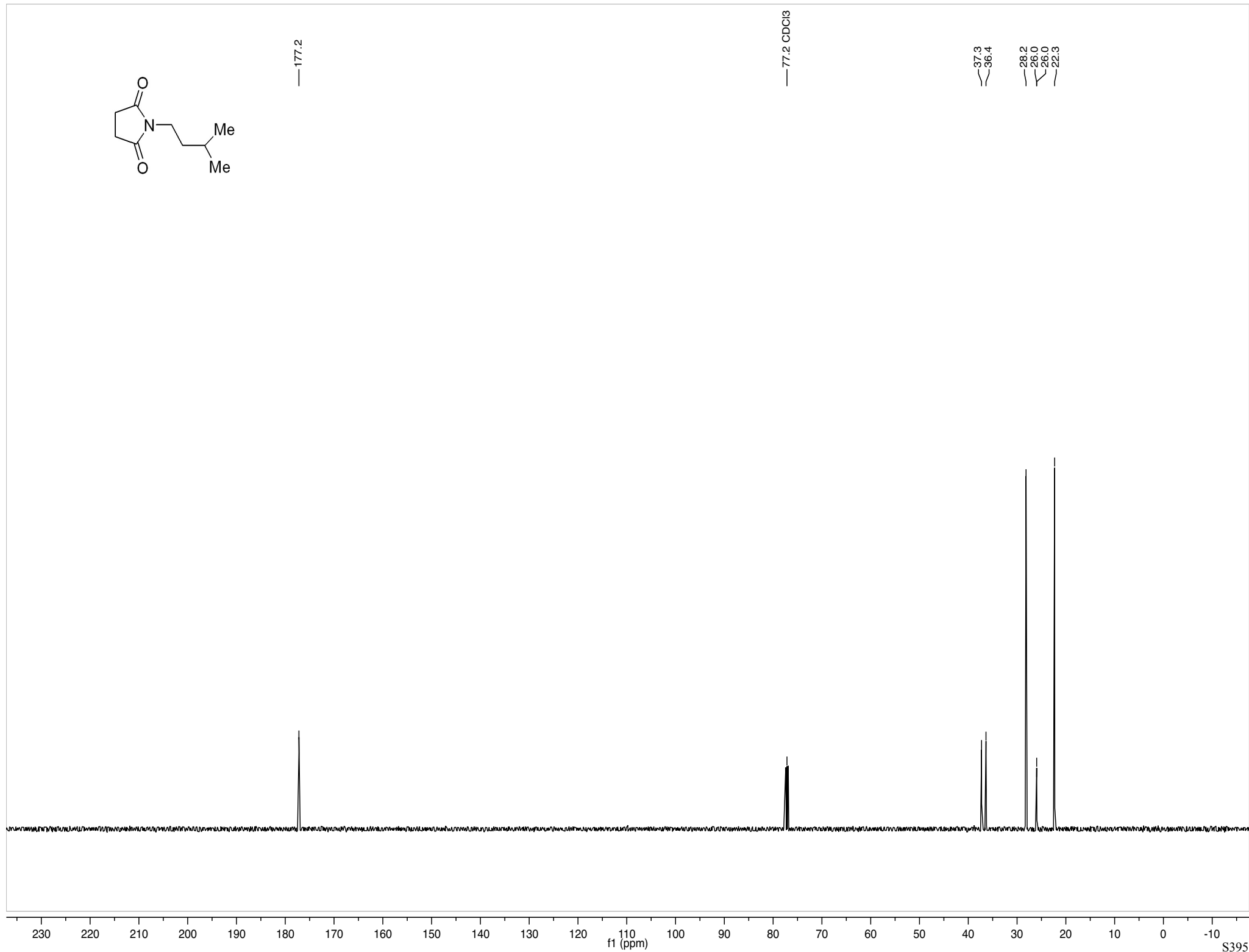


— 177.2

— 77.2 CDCl₃

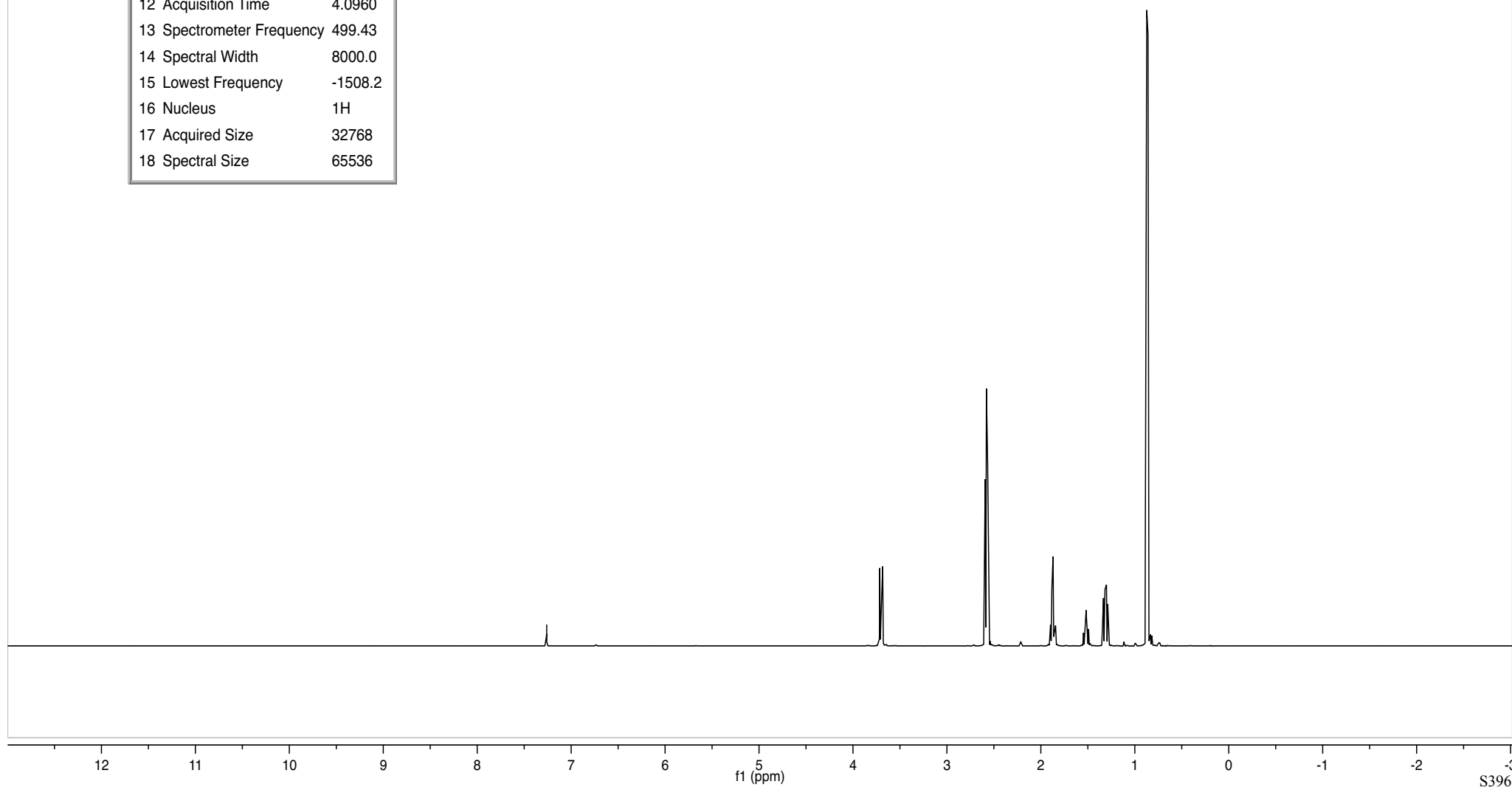
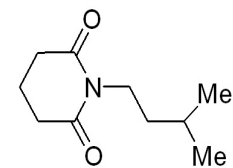
37.3
36.4

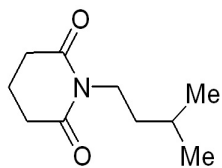
28.2
26.0
26.0
22.3



	Parameter	Value
1	Origin	Varian
2	Spectrometer	inova
3	Solvent	CDCl ₃
4	Temperature	20.0
5	Pulse Sequence	s2pul
6	Experiment	1D
7	Probe	QUADG
8	Number of Scans	8
9	Receiver Gain	44
10	Relaxation Delay	0.0000
11	Pulse Width	0.0000
12	Acquisition Time	4.0960
13	Spectrometer Frequency	499.43
14	Spectral Width	8000.0
15	Lowest Frequency	-1508.2
16	Nucleus	¹ H
17	Acquired Size	32768
18	Spectral Size	65536

— 7.26 CDCl₃





— 7.26 CDCl₃

3.71
3.70
3.70
3.69
3.68

2.59
2.58
2.57

1.90
1.88
1.87
1.86
1.84
1.57
1.56
1.55
1.53
1.52
1.51
1.49
1.48
1.47
1.33
1.32
1.32
1.31
1.31
1.30
1.30
1.29
0.87
0.86



2.00
4.00
2.03
0.98
2.01
6.04

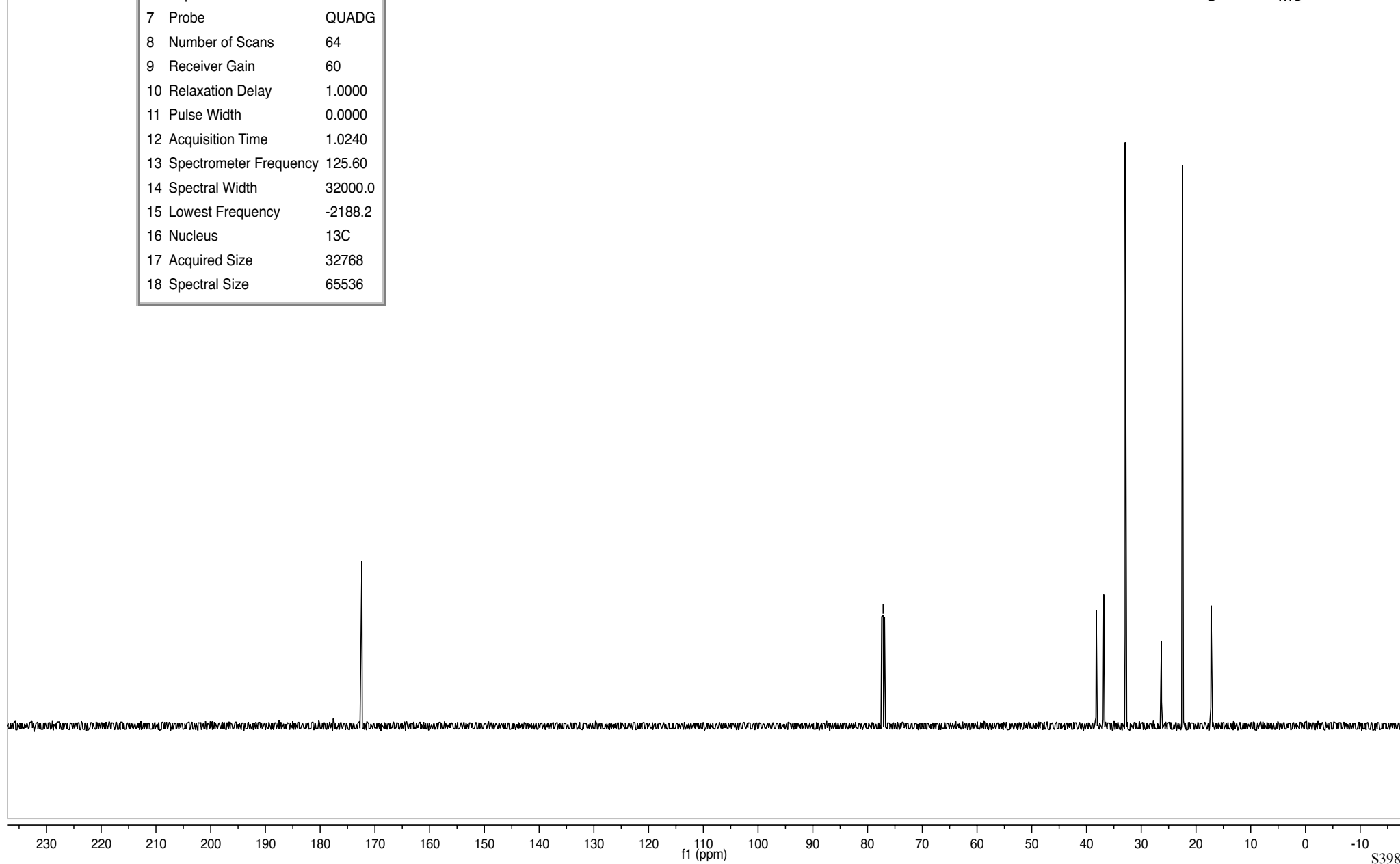
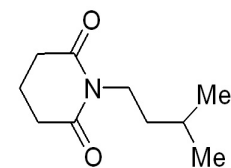
12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2

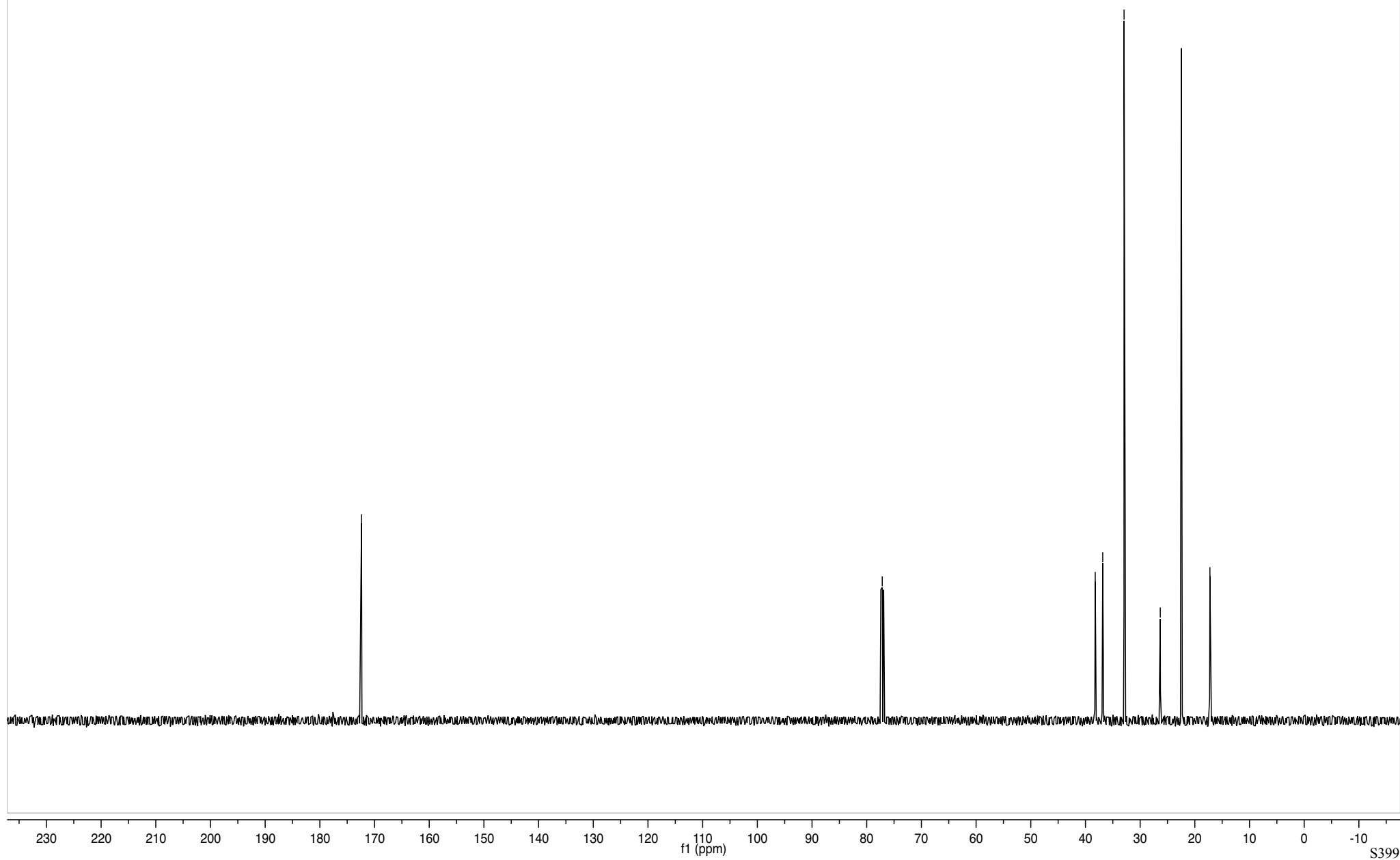
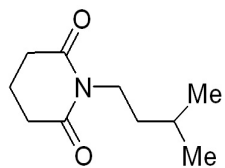
f1 (ppm)

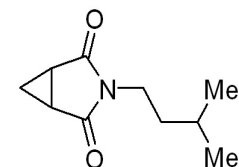
S397

	Parameter	Value
1	Origin	Varian
2	Spectrometer	inova
3	Solvent	CDCl3
4	Temperature	20.0
5	Pulse Sequence	s2pul
6	Experiment	1D
7	Probe	QUADG
8	Number of Scans	64
9	Receiver Gain	60
10	Relaxation Delay	1.0000
11	Pulse Width	0.0000
12	Acquisition Time	1.0240
13	Spectrometer Frequency	125.60
14	Spectral Width	32000.0
15	Lowest Frequency	-2188.2
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

— 77.16 CDCl3



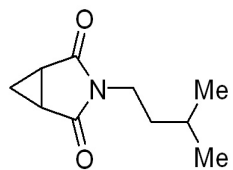




— 7.26 CDCl₃

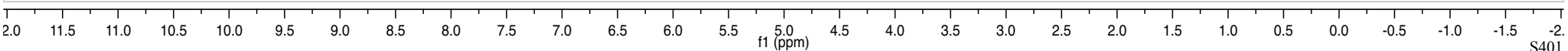
	Parameter	Value
1	Origin	Varian
2	Spectrometer	inova
3	Solvent	CDCl ₃
4	Temperature	20.0
5	Pulse Sequence	s2pul
6	Experiment	1D
7	Probe	QUAD
8	Number of Scans	8
9	Receiver Gain	41
10	Relaxation Delay	0.0000
11	Pulse Width	0.0000
12	Acquisition Time	4.6645
13	Spectrometer Frequency	499.69
14	Spectral Width	7024.9
15	Lowest Frequency	-1011.9
16	Nucleus	¹ H
17	Acquired Size	32768
18	Spectral Size	65536

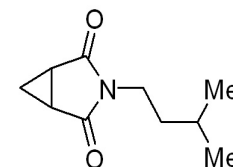
2.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm) S400



— 7.26 CDCl₃

3.36
3.35
3.34
3.34
3.33
2.45
2.44
2.43
2.42
1.54
1.53
1.52
1.51
1.50
1.49
1.49
1.48
1.47
1.46
1.45
1.43
1.36
1.35
1.34
1.33
1.33
1.32
1.31
1.31
1.30
1.30
0.90
0.88

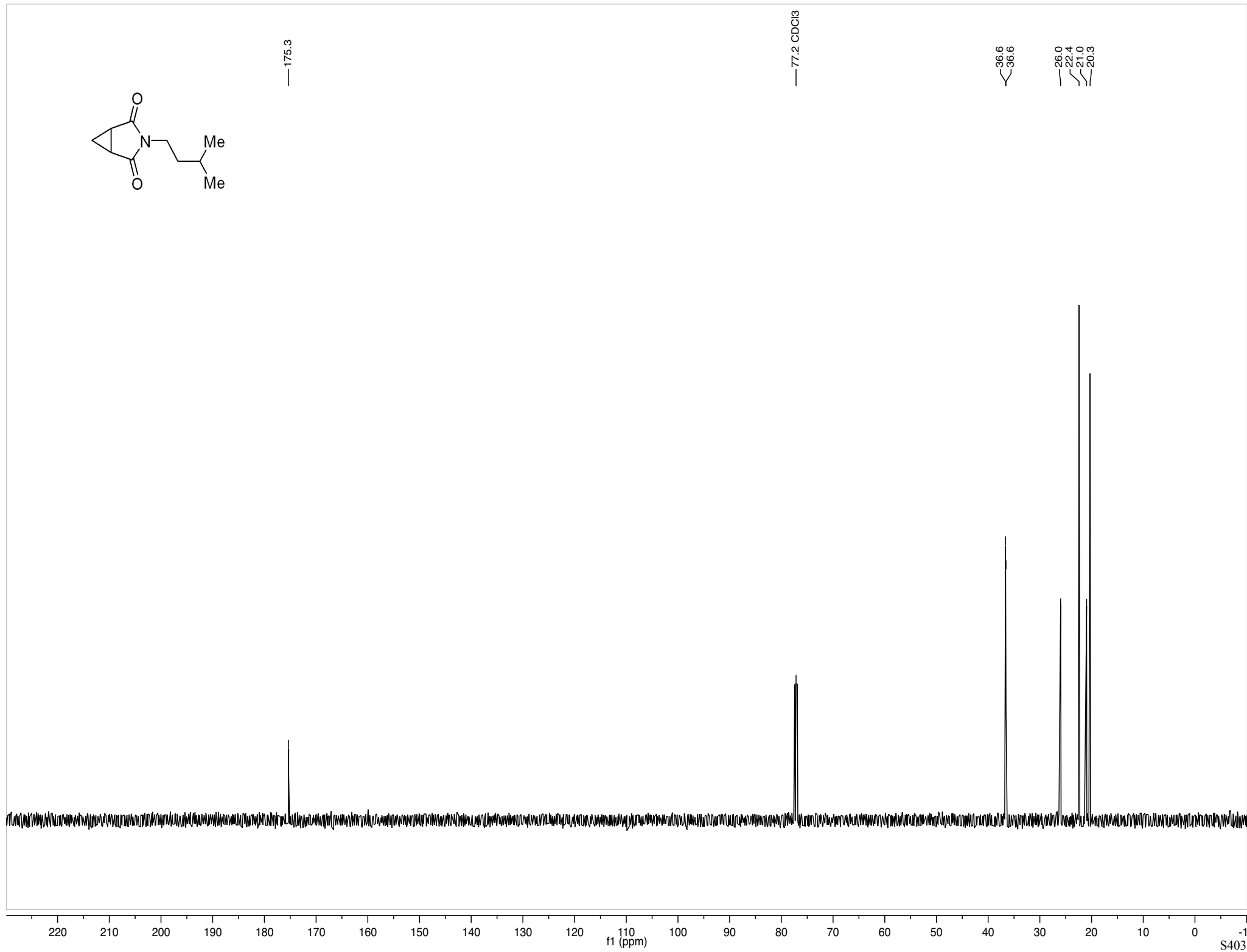
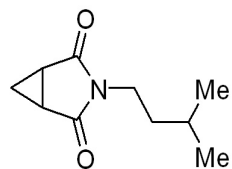




— 77.2 CDCl₃

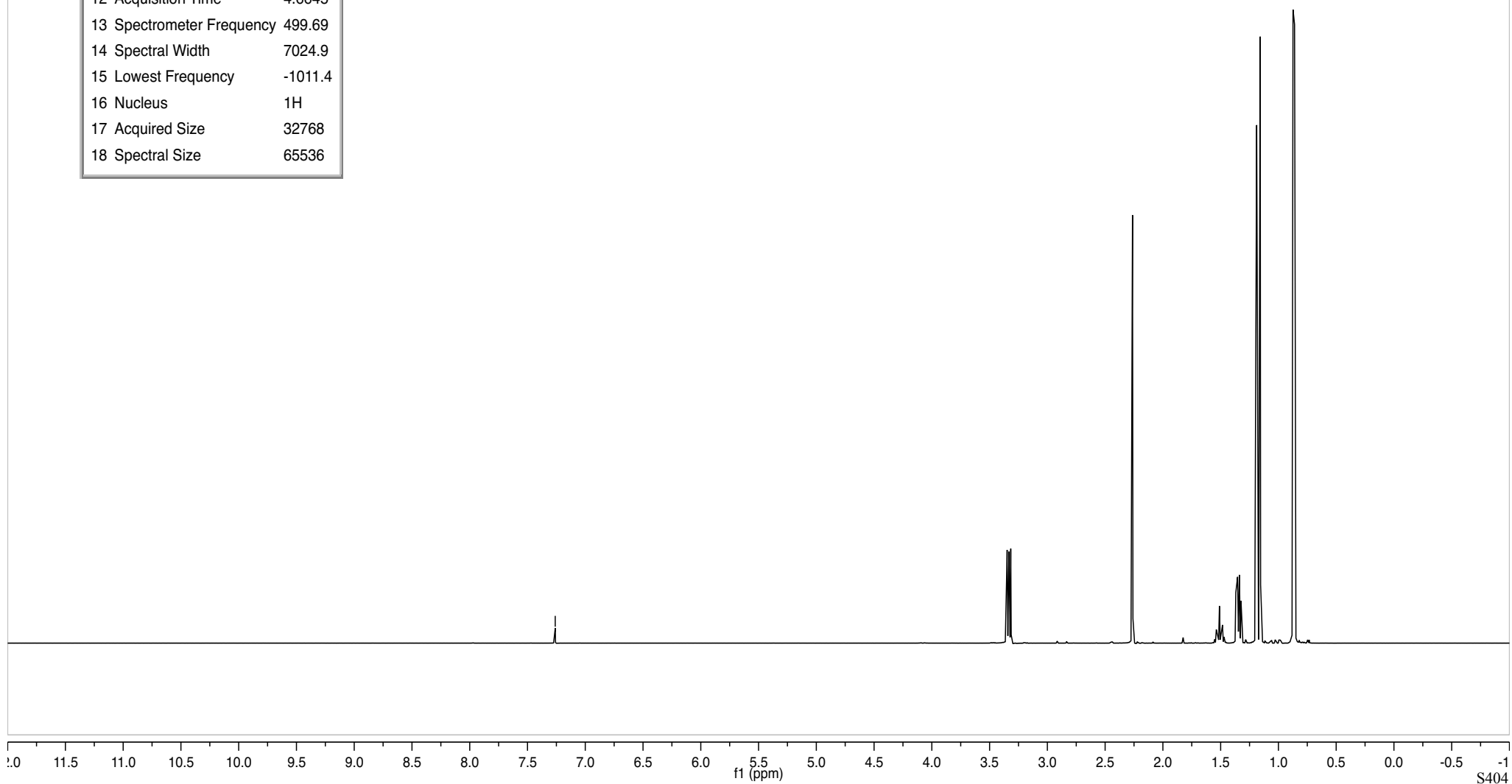
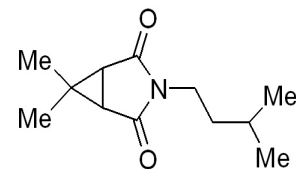
	Parameter	Value
1	Origin	Varian
2	Spectrometer	inova
3	Solvent	CDCl ₃
4	Temperature	20.0
5	Pulse Sequence	s2pul
6	Experiment	1D
7	Probe	QUAD
8	Number of Scans	64
9	Receiver Gain	60
10	Relaxation Delay	1.0000
11	Pulse Width	0.0000
12	Acquisition Time	1.0863
13	Spectrometer Frequency	125.66
14	Spectral Width	30165.9
15	Lowest Frequency	-1260.2
16	Nucleus	¹³ C
17	Acquired Size	32768
18	Spectral Size	65536

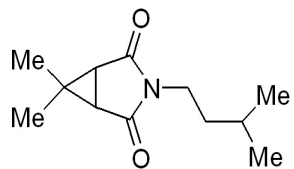
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm) S402



	Parameter	Value
1	Origin	Varian
2	Spectrometer	inova
3	Solvent	CDCl3
4	Temperature	20.0
5	Pulse Sequence	s2pul
6	Experiment	1D
7	Probe	QUAD
8	Number of Scans	8
9	Receiver Gain	30
10	Relaxation Delay	0.0000
11	Pulse Width	0.0000
12	Acquisition Time	4.6645
13	Spectrometer Frequency	499.69
14	Spectral Width	7024.9
15	Lowest Frequency	-1011.4
16	Nucleus	¹ H
17	Acquired Size	32768
18	Spectral Size	65536

— 7.26 CDCl₃





7.26 CDCl₃

3.35
3.34
3.33
3.32

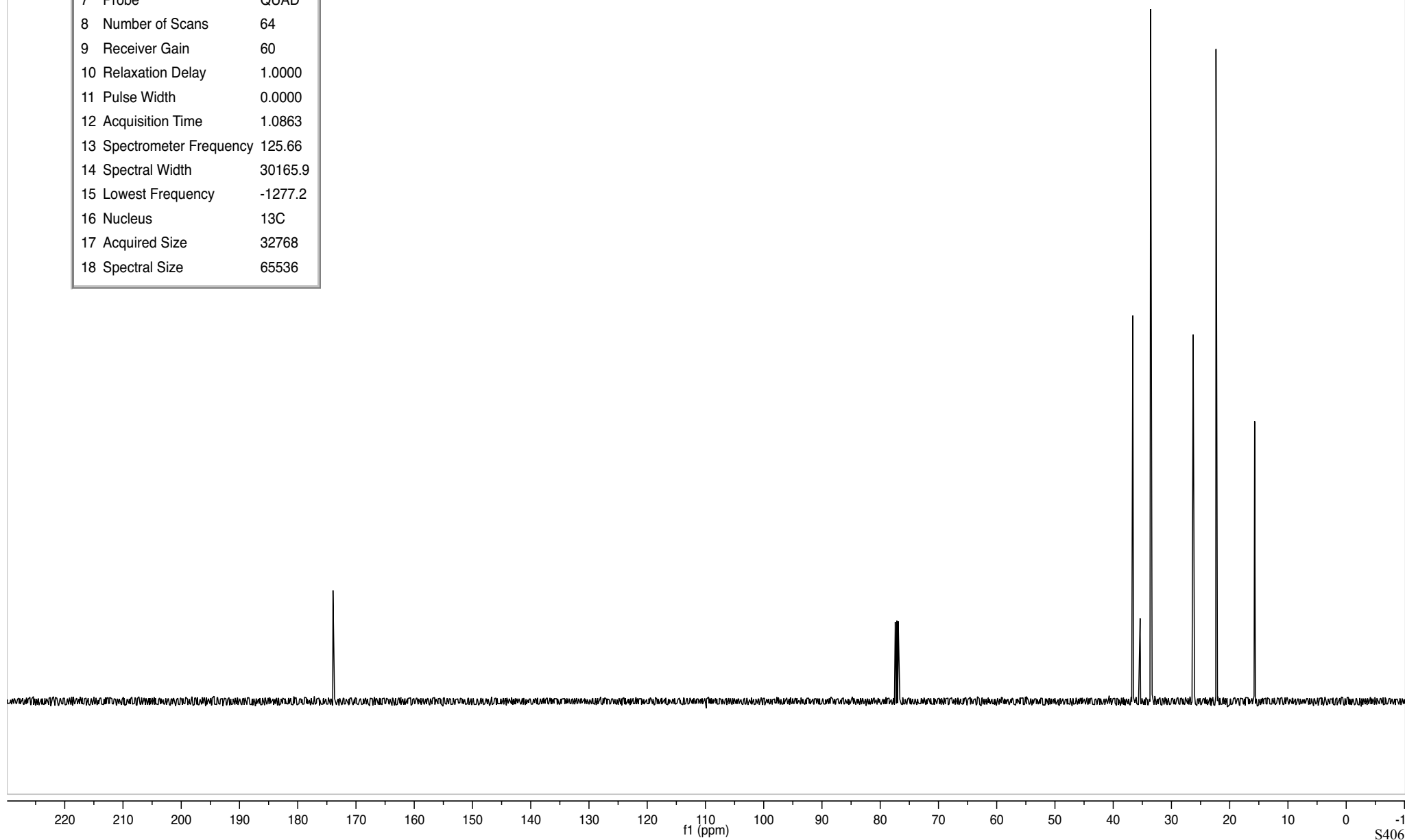
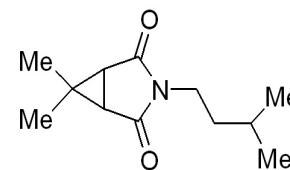
2.26
1.37
1.36
1.35
1.34
1.34
1.34
1.32
1.19
1.18
1.16
1.15
0.87
0.86

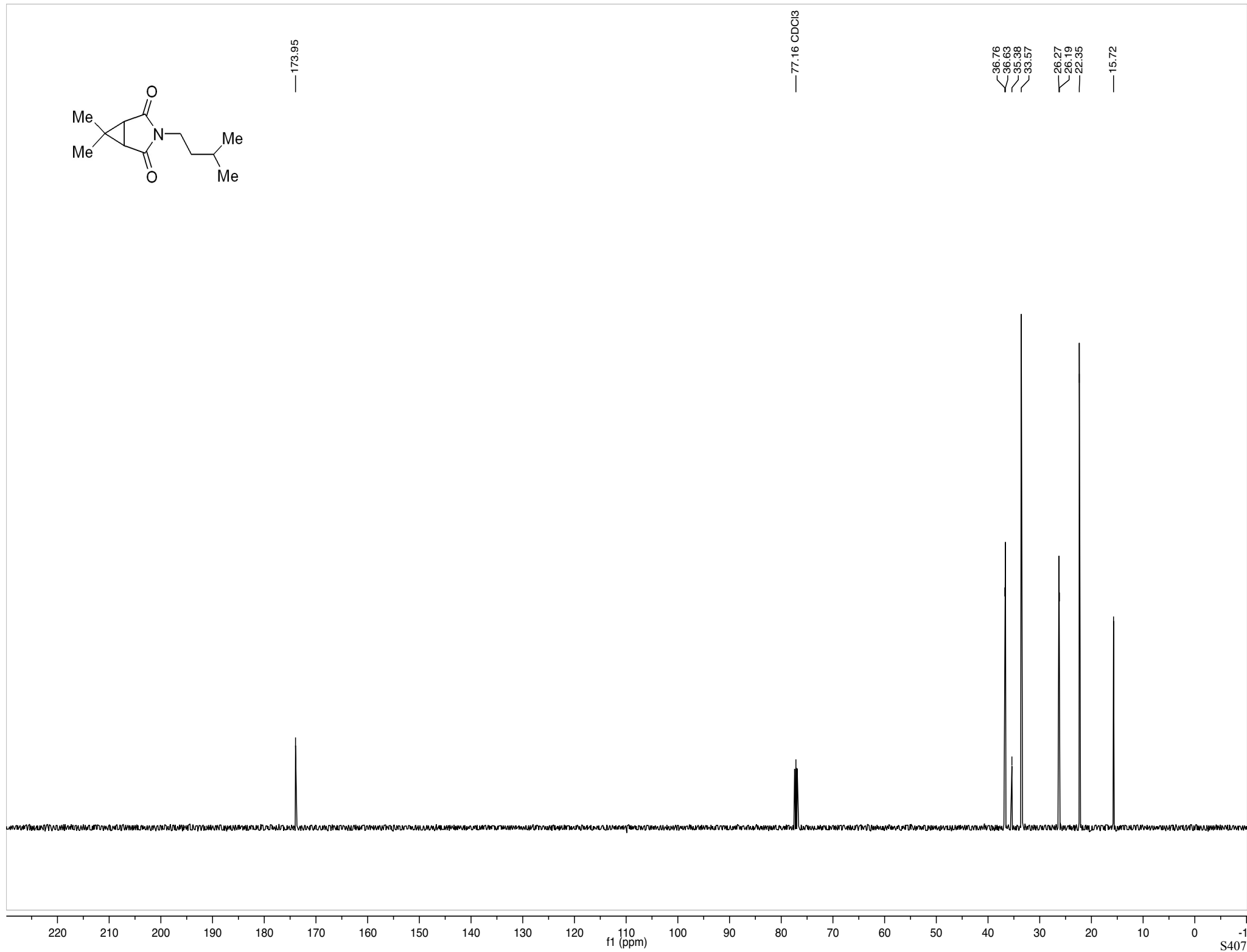
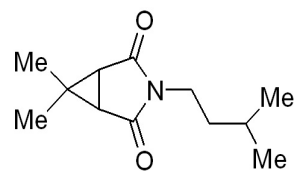
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0

f1 (ppm)

S405

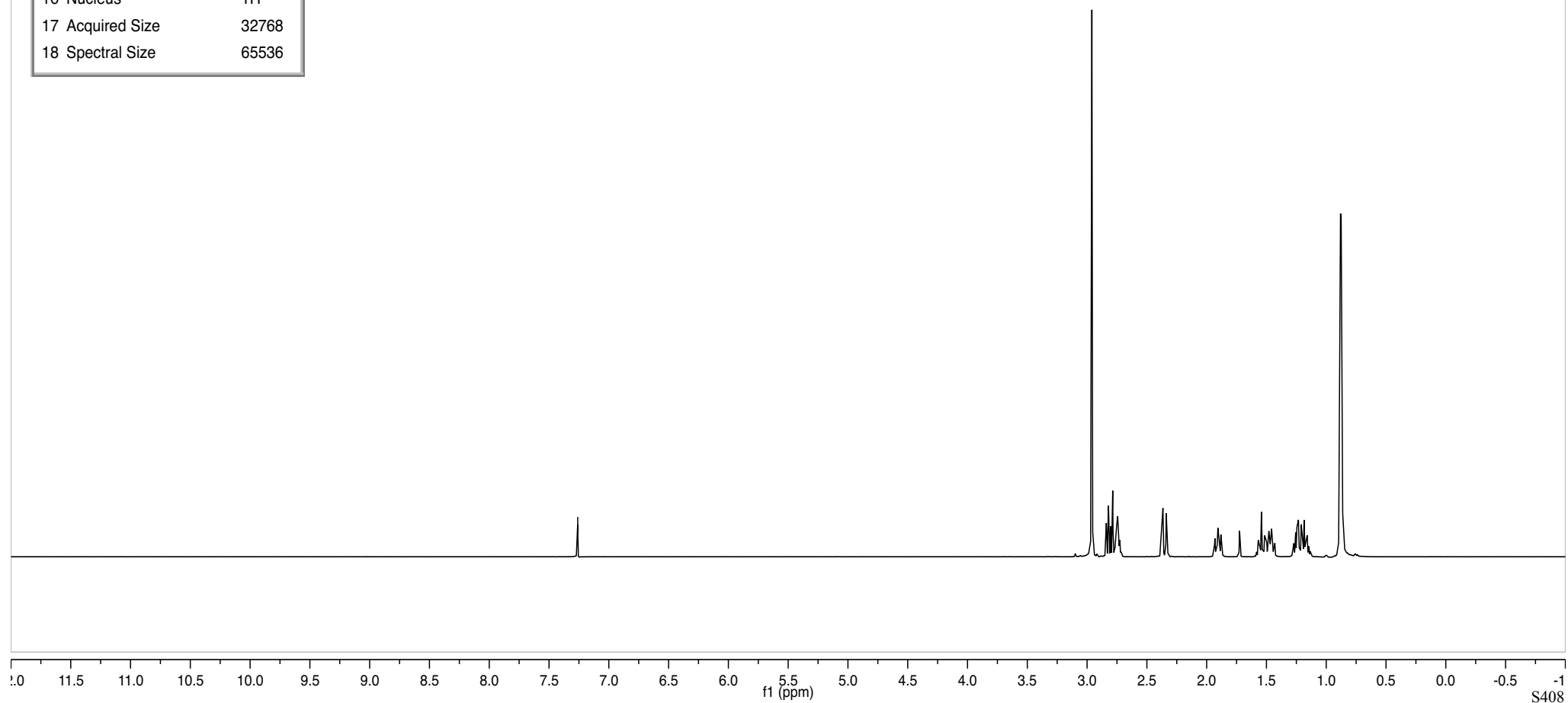
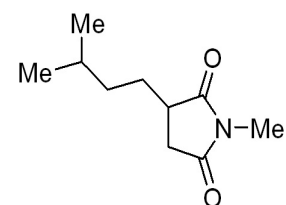
	Parameter	Value
1	Origin	Varian
2	Spectrometer	inova
3	Solvent	CDCl3
4	Temperature	20.0
5	Pulse Sequence	s2pul
6	Experiment	1D
7	Probe	QUAD
8	Number of Scans	64
9	Receiver Gain	60
10	Relaxation Delay	1.0000
11	Pulse Width	0.0000
12	Acquisition Time	1.0863
13	Spectrometer Frequency	125.66
14	Spectral Width	30165.9
15	Lowest Frequency	-1277.2
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

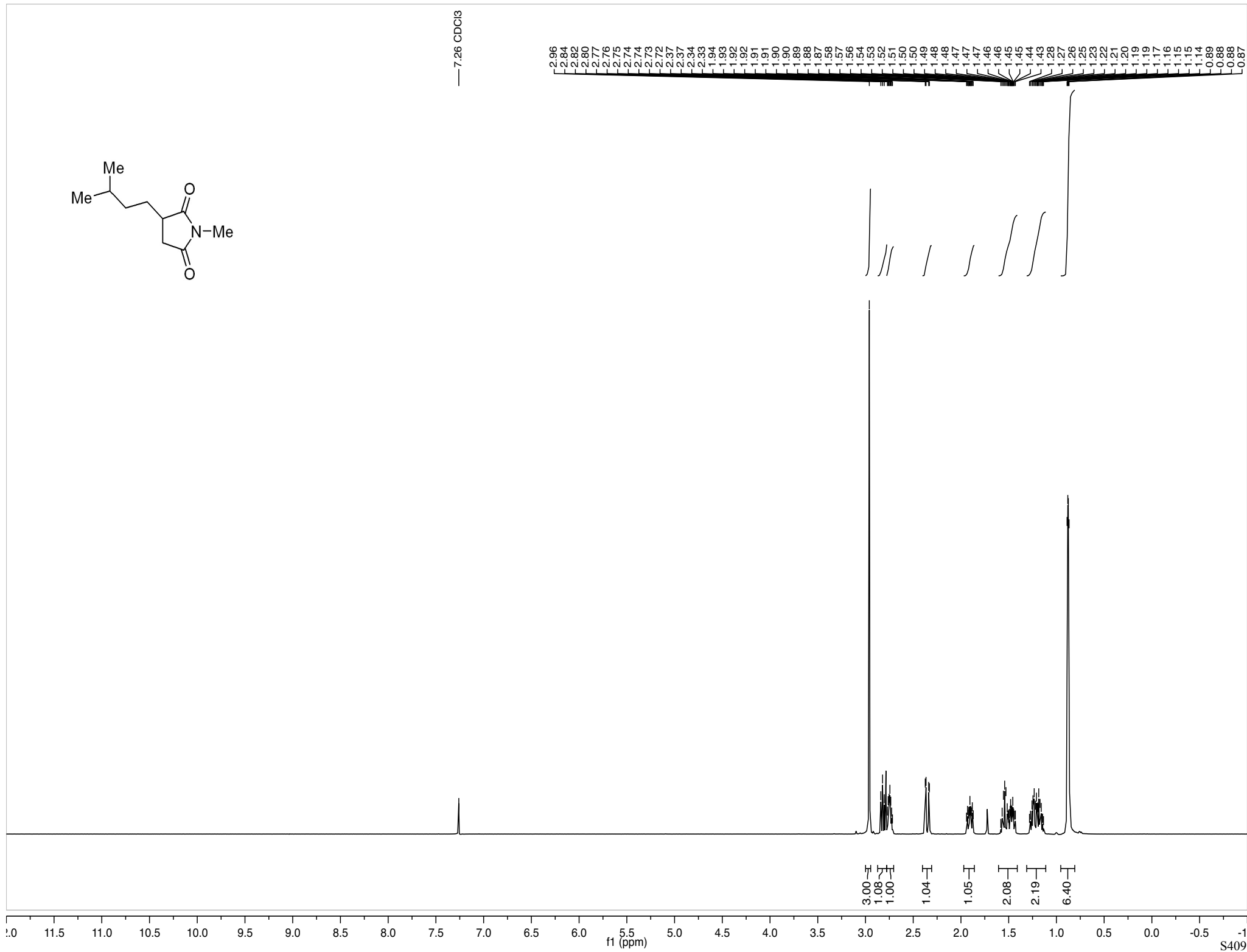




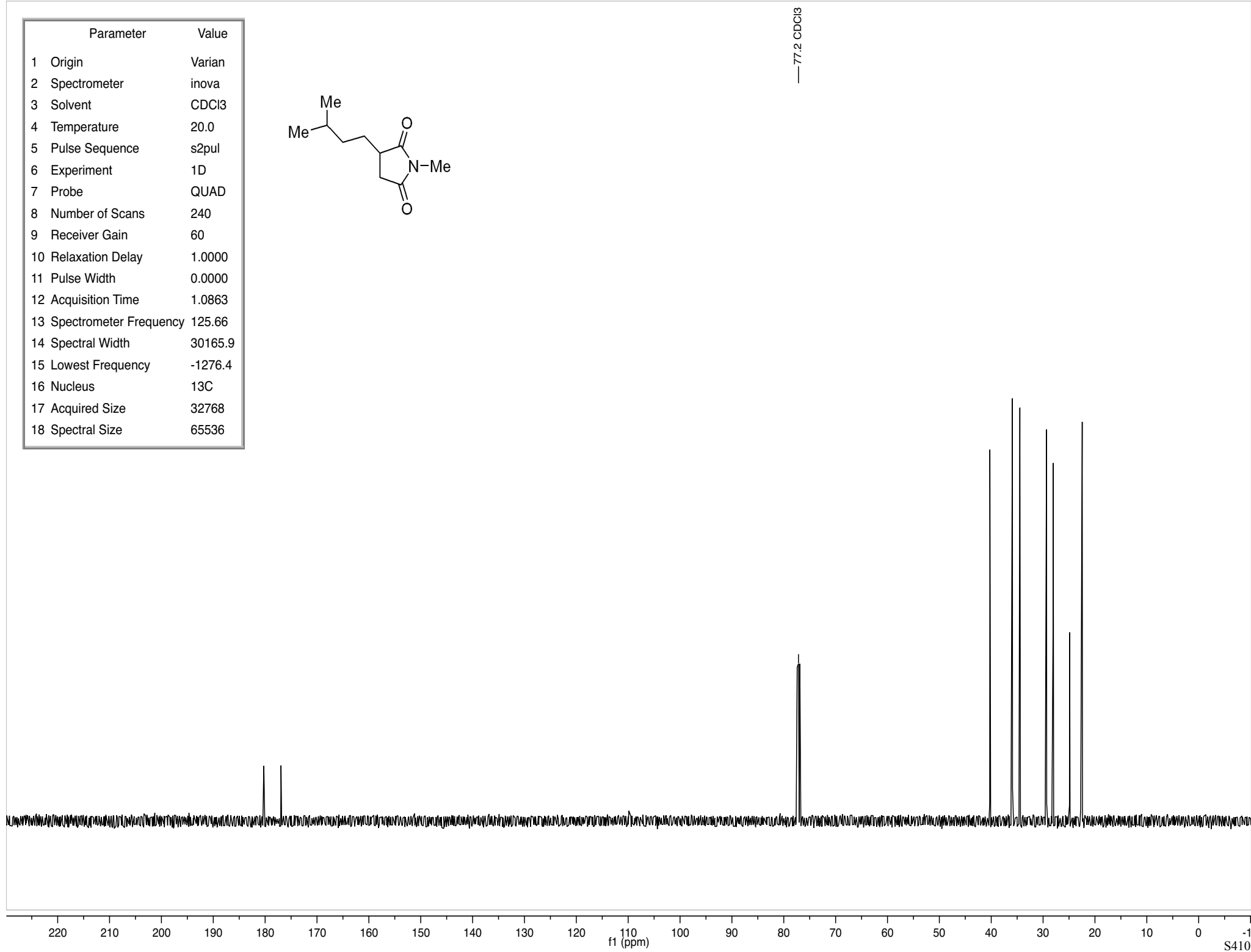
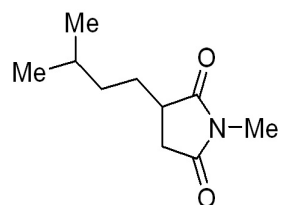
Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	8
9 Receiver Gain	41
10 Relaxation Delay	0.0000
11 Pulse Width	0.0000
12 Acquisition Time	4.6645
13 Spectrometer Frequency	499.69
14 Spectral Width	7024.9
15 Lowest Frequency	-1021.4
16 Nucleus	1H
17 Acquired Size	32768
18 Spectral Size	65536

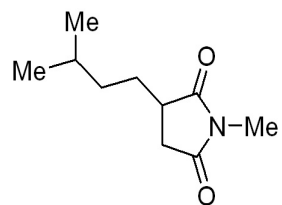
— 7.3 CDCl3





Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	240
9 Receiver Gain	60
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.0863
13 Spectrometer Frequency	125.66
14 Spectral Width	30165.9
15 Lowest Frequency	-1276.4
16 Nucleus	¹³ C
17 Acquired Size	32768
18 Spectral Size	65536

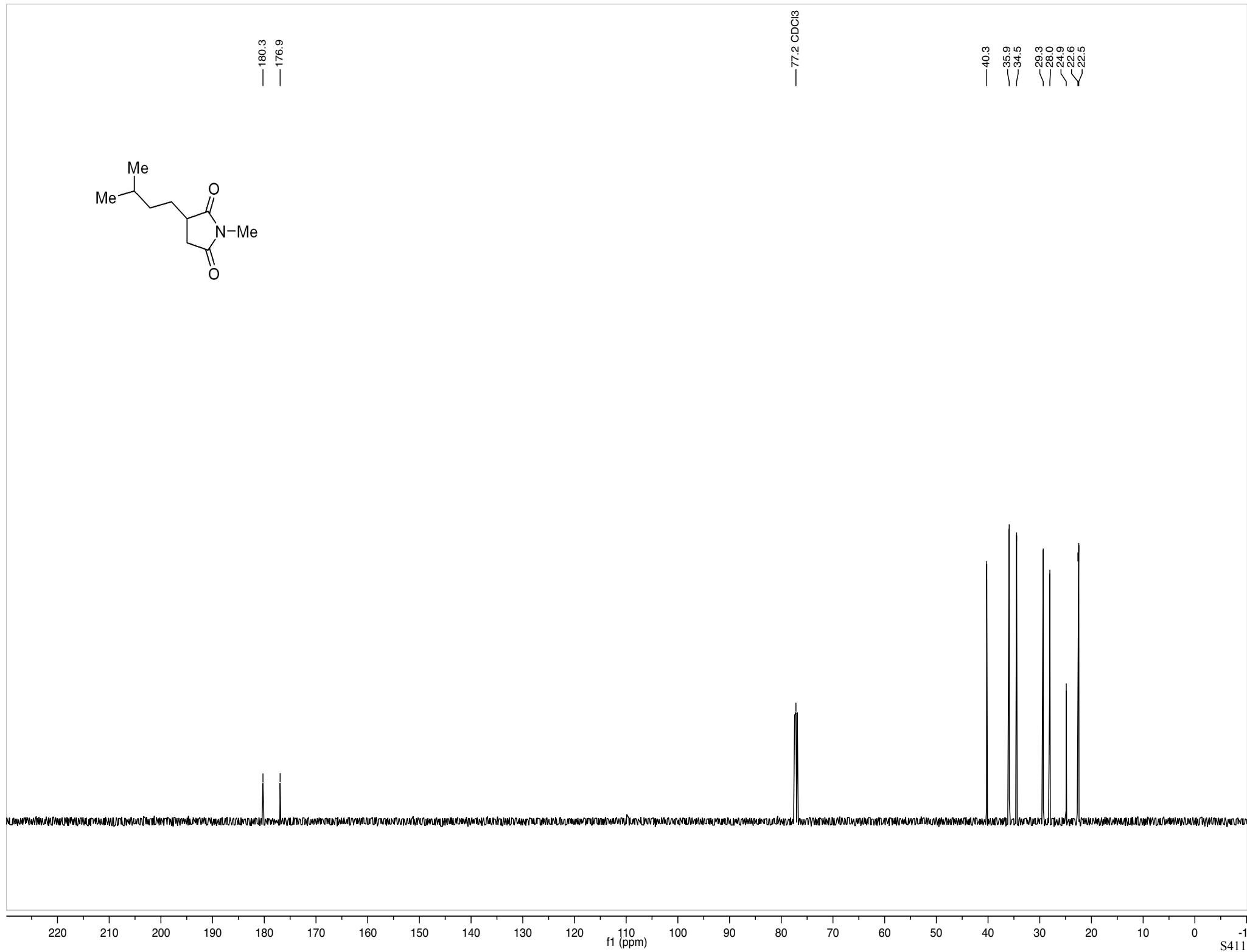




— 180.3
— 176.9

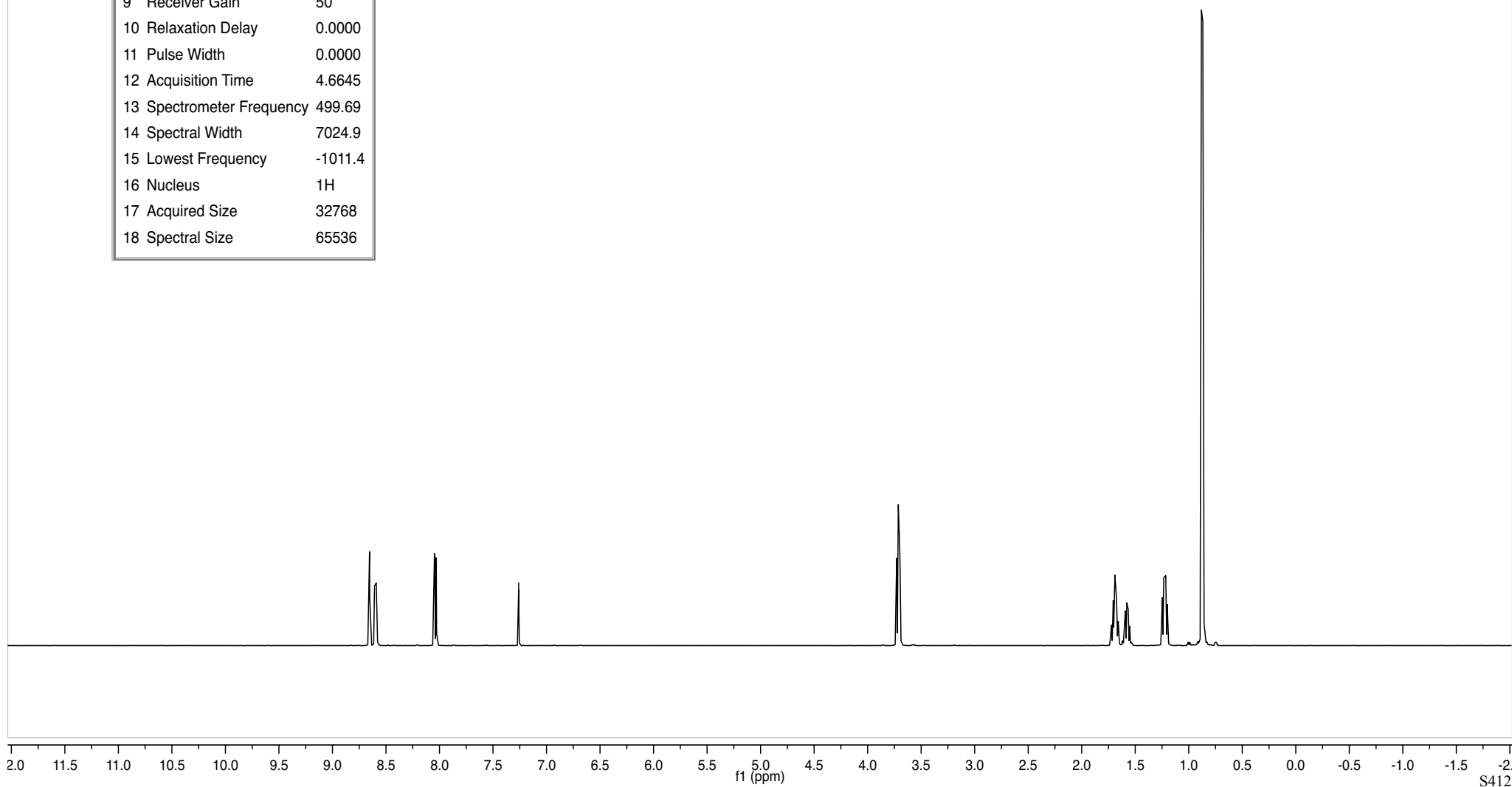
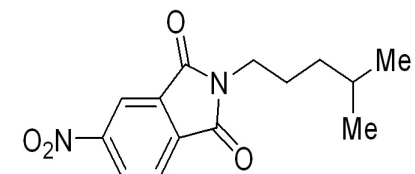
— 77.2 CDCl₃

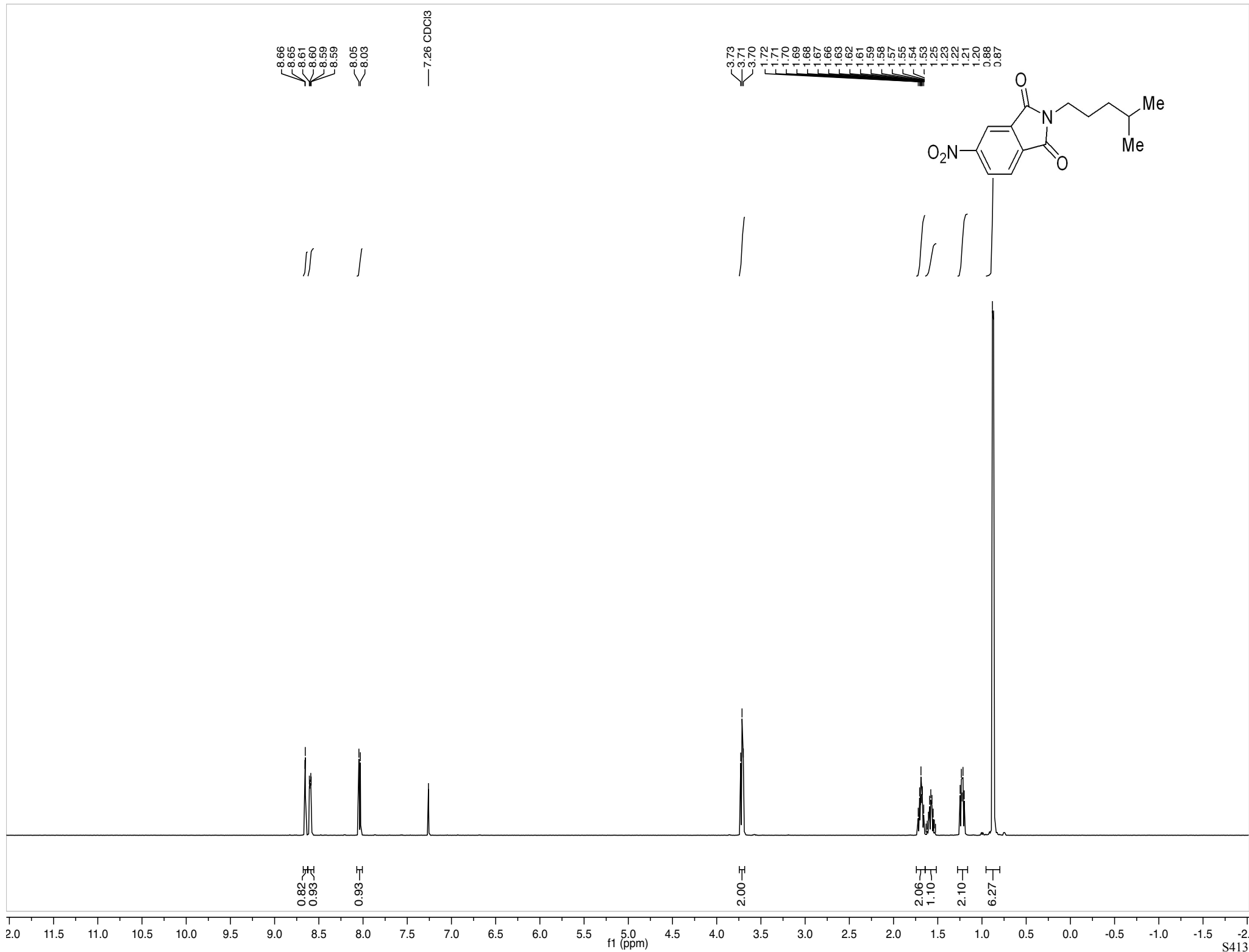
— 40.3
— 35.9
— 34.5
— 29.3
— 28.0
— 24.9
— 22.6
— 22.5



	Parameter	Value
1	Origin	Varian
2	Spectrometer	inova
3	Solvent	CDCl3
4	Temperature	40.0
5	Pulse Sequence	s2pul
6	Experiment	1D
7	Probe	QUAD
8	Number of Scans	8
9	Receiver Gain	50
10	Relaxation Delay	0.0000
11	Pulse Width	0.0000
12	Acquisition Time	4.6645
13	Spectrometer Frequency	499.69
14	Spectral Width	7024.9
15	Lowest Frequency	-1011.4
16	Nucleus	¹ H
17	Acquired Size	32768
18	Spectral Size	65536

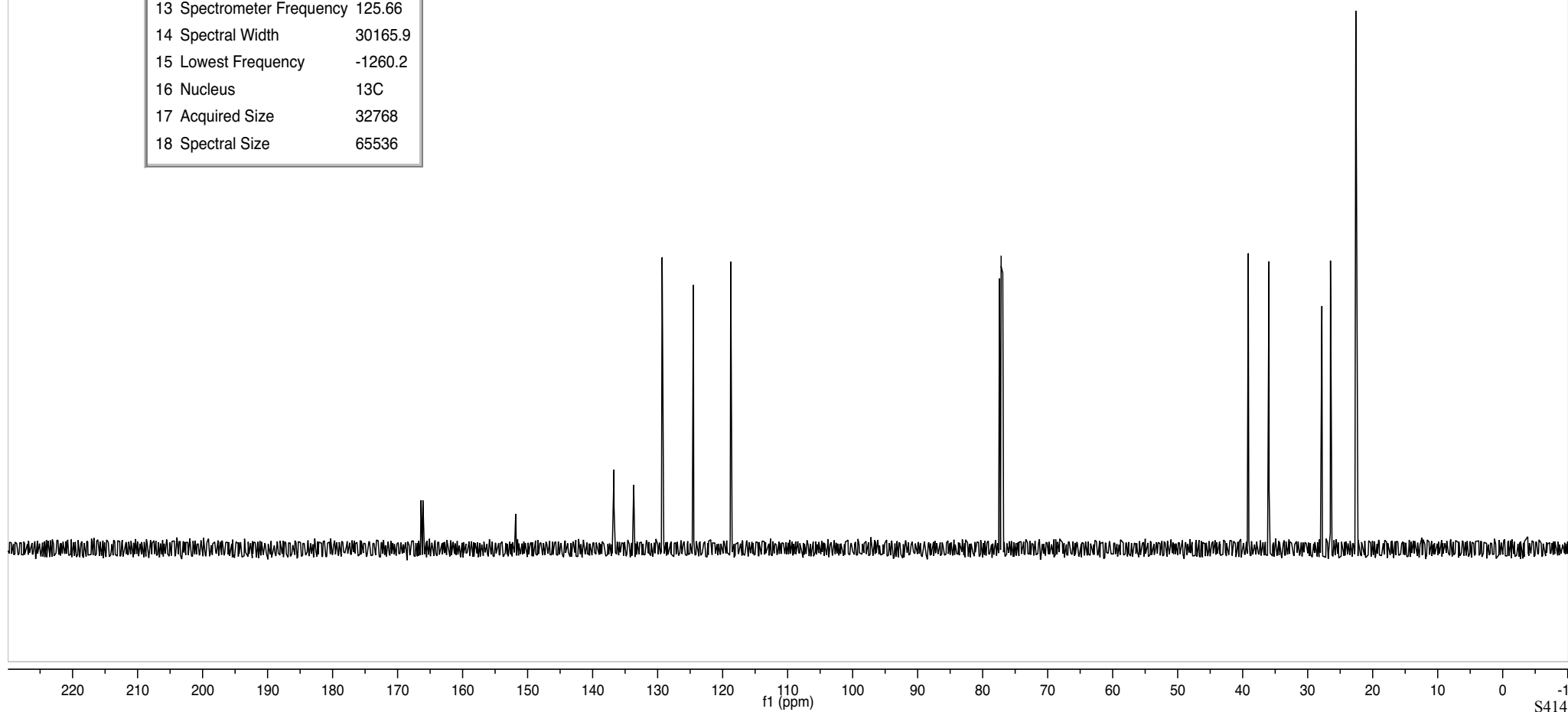
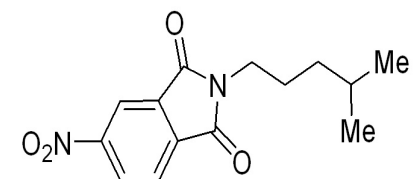
— 7.26 CDCl₃

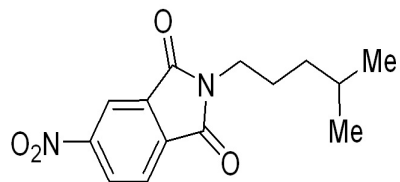




	Parameter	Value
1	Origin	Varian
2	Spectrometer	inova
3	Solvent	CDCl3
4	Temperature	40.0
5	Pulse Sequence	s2pul
6	Experiment	1D
7	Probe	QUAD
8	Number of Scans	224
9	Receiver Gain	60
10	Relaxation Delay	1.0000
11	Pulse Width	0.0000
12	Acquisition Time	1.0863
13	Spectrometer Frequency	125.66
14	Spectral Width	30165.9
15	Lowest Frequency	-1260.2
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

— 77.16 CDCl3





166.4
166.1

151.8

136.7

133.7

129.3

124.5

118.8

77.2 CDCl₃

39.1

35.9

27.8

26.5

22.6

220

210

200

190

180

170

160

150

140

130

120

110

100

90

80

70

60

50

40

30

20

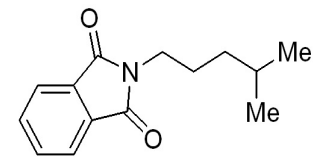
10

0

-1

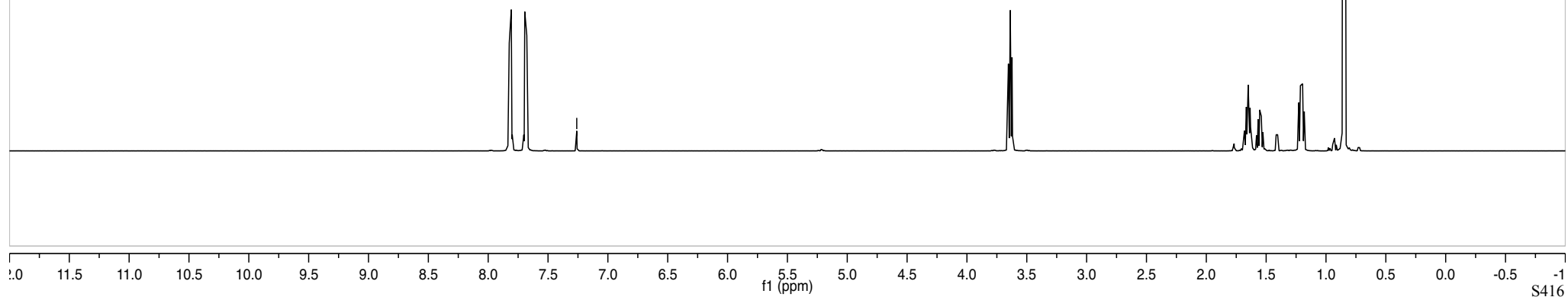
f1 (ppm)

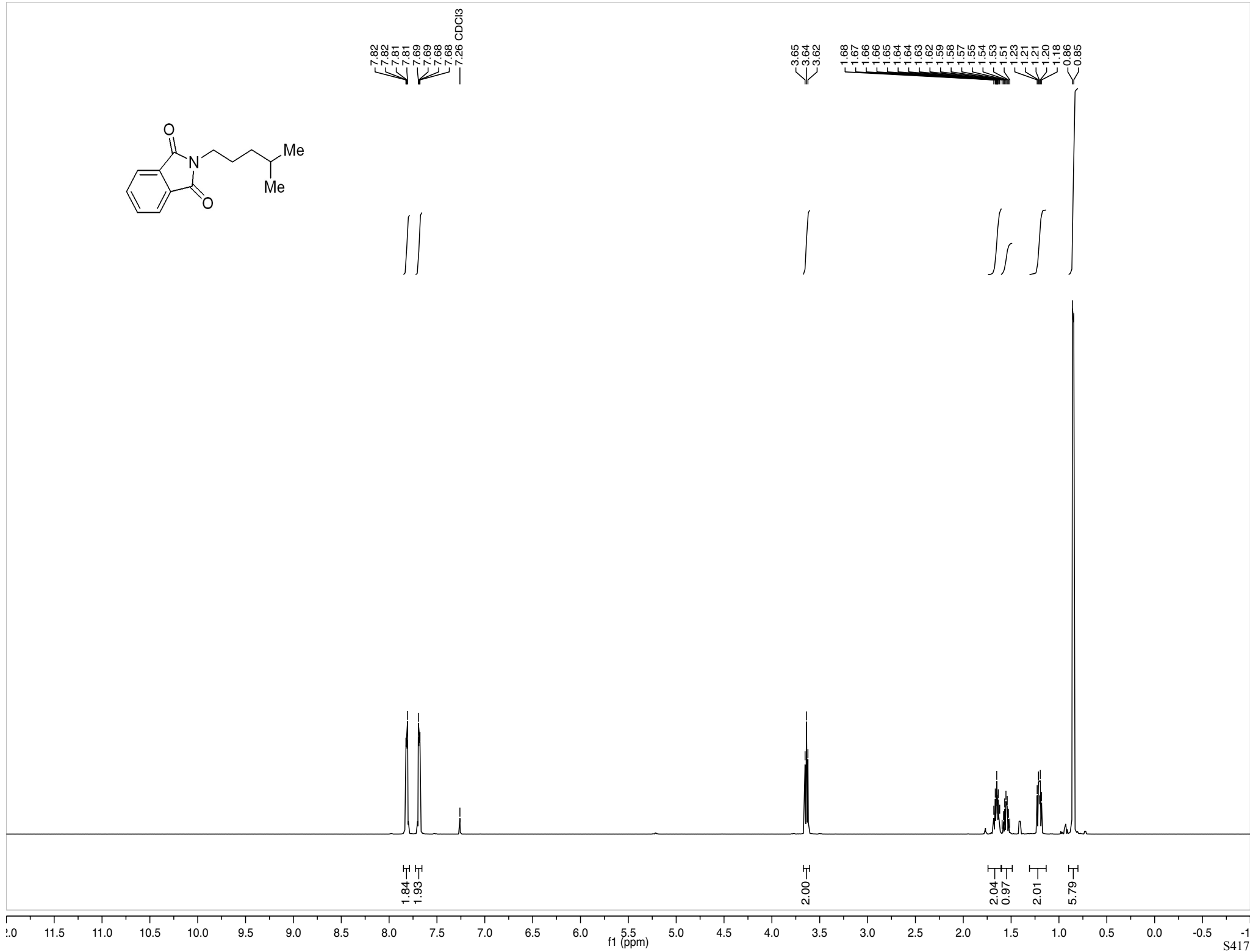
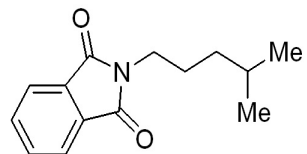
S415



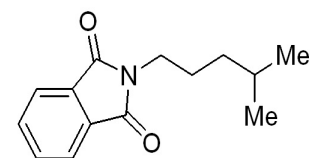
— 7.26 CDCl₃

Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl ₃
4 Temperature	40.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	8
9 Receiver Gain	41
10 Relaxation Delay	0.0000
11 Pulse Width	0.0000
12 Acquisition Time	4.6645
13 Spectrometer Frequency	499.69
14 Spectral Width	7024.9
15 Lowest Frequency	-1011.4
16 Nucleus	¹ H
17 Acquired Size	32768
18 Spectral Size	65536

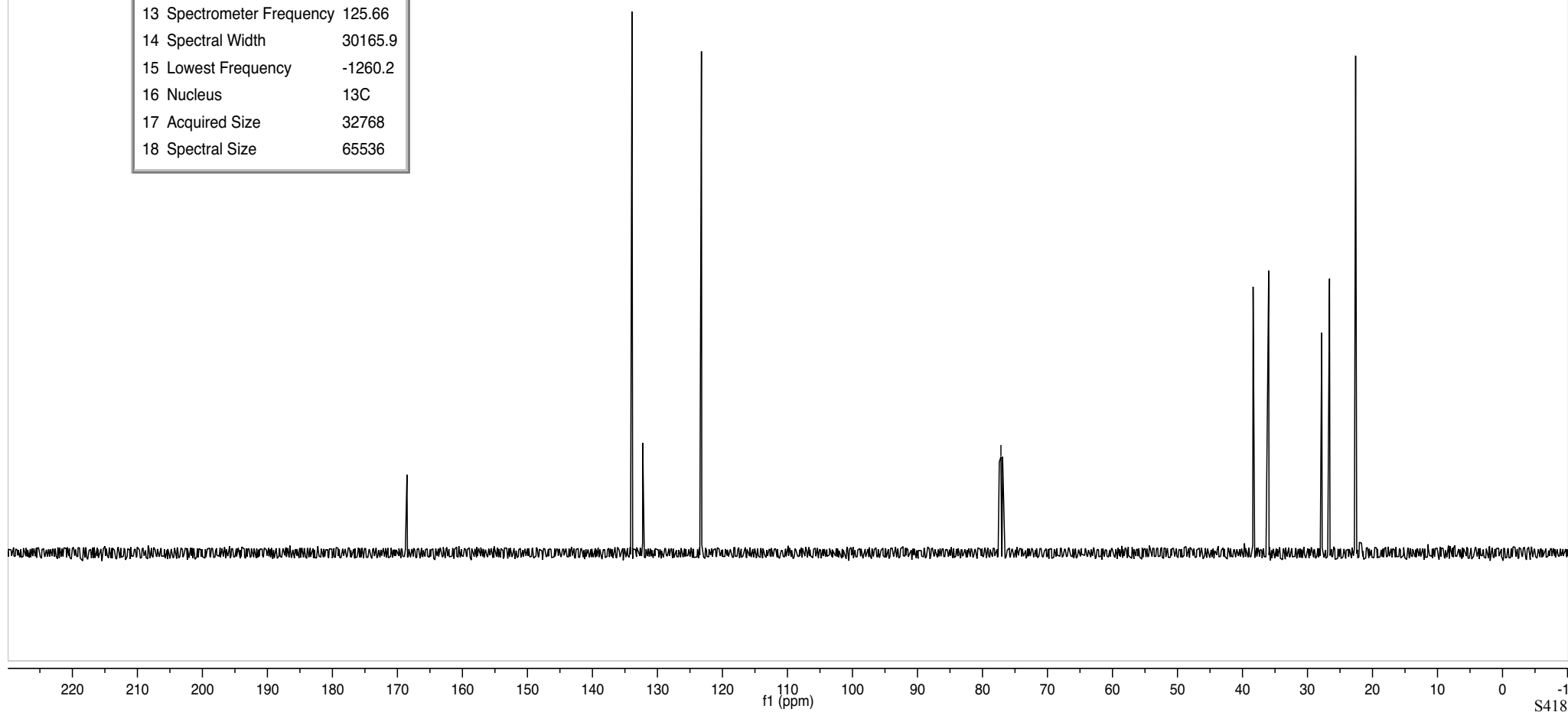


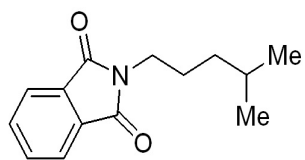


	Parameter	Value
1	Origin	Varian
2	Spectrometer	inova
3	Solvent	CDCl3
4	Temperature	40.0
5	Pulse Sequence	s2pul
6	Experiment	1D
7	Probe	QUAD
8	Number of Scans	48
9	Receiver Gain	60
10	Relaxation Delay	1.0000
11	Pulse Width	0.0000
12	Acquisition Time	1.0863
13	Spectrometer Frequency	125.66
14	Spectral Width	30165.9
15	Lowest Frequency	-1260.2
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536



— 77.2 CDCl3





— 168.5

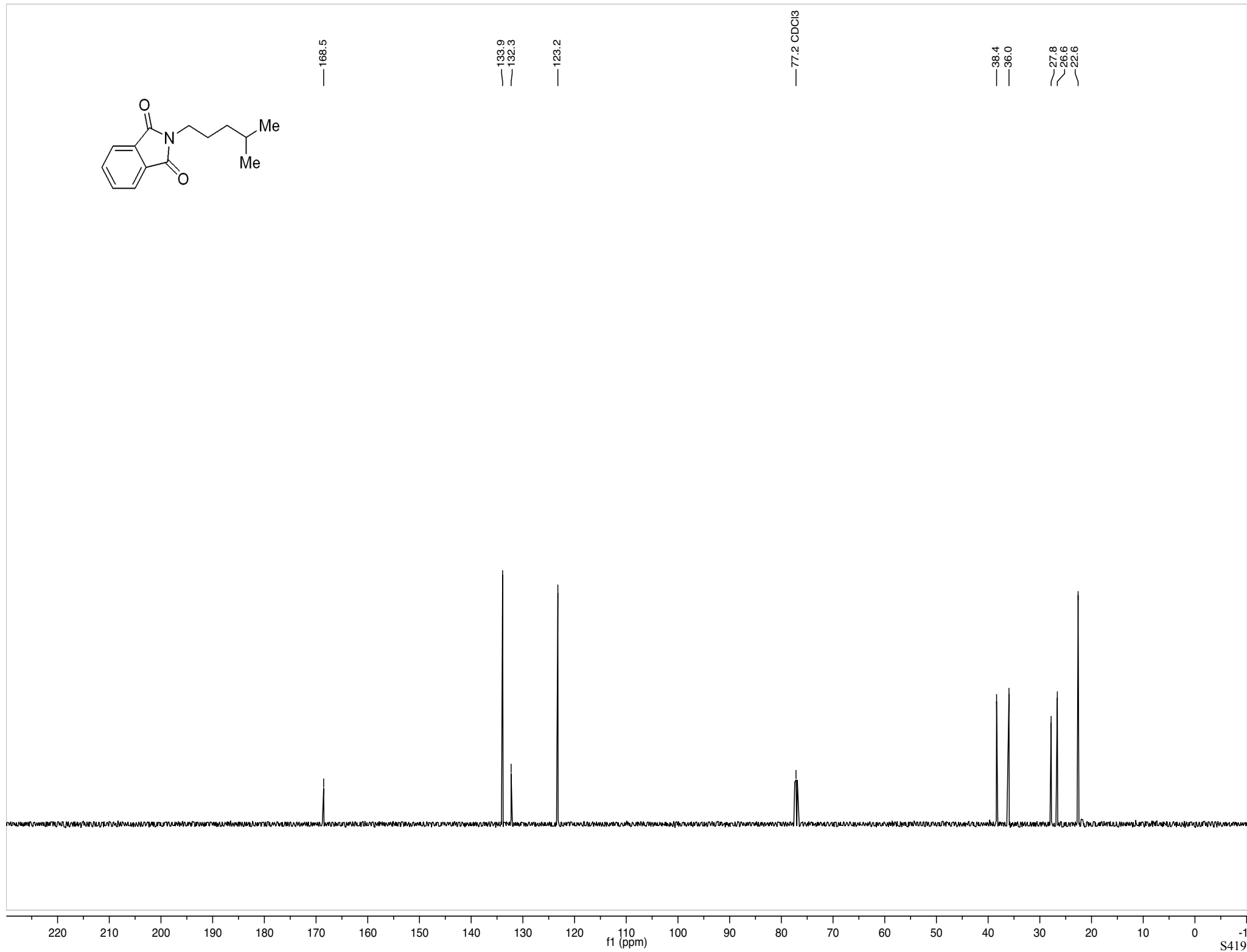
— 133.9
— 132.3

— 123.2

— 77.2 CDCl₃

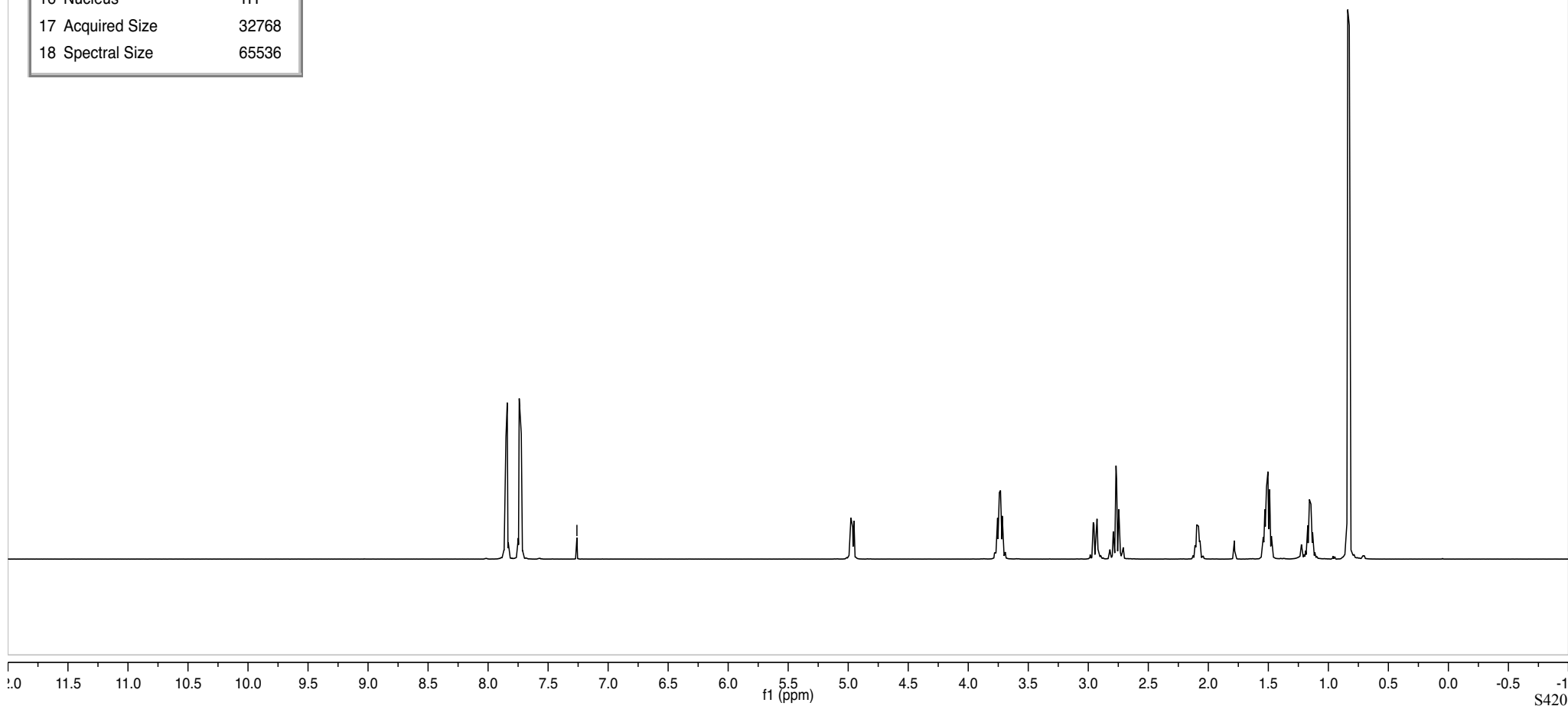
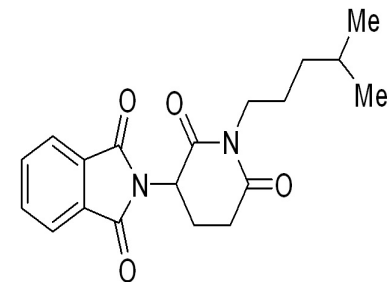
— 38.4
— 36.0

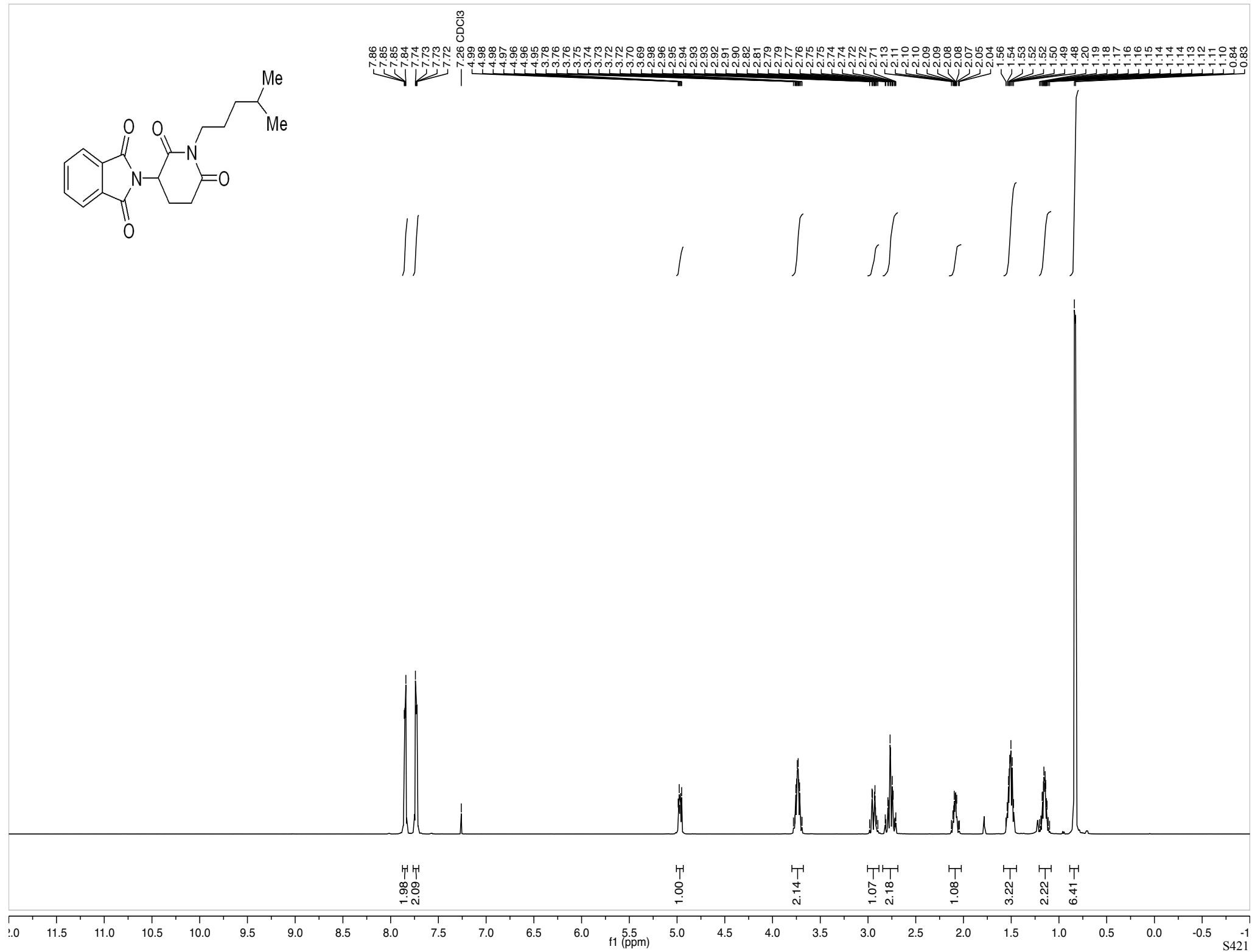
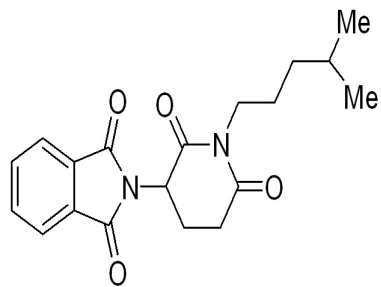
— 27.8
— 26.6
— 22.6



Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	8
9 Receiver Gain	36
10 Relaxation Delay	0.0000
11 Pulse Width	0.0000
12 Acquisition Time	4.6645
13 Spectrometer Frequency	499.69
14 Spectral Width	7024.9
15 Lowest Frequency	-1021.4
16 Nucleus	¹ H
17 Acquired Size	32768
18 Spectral Size	65536

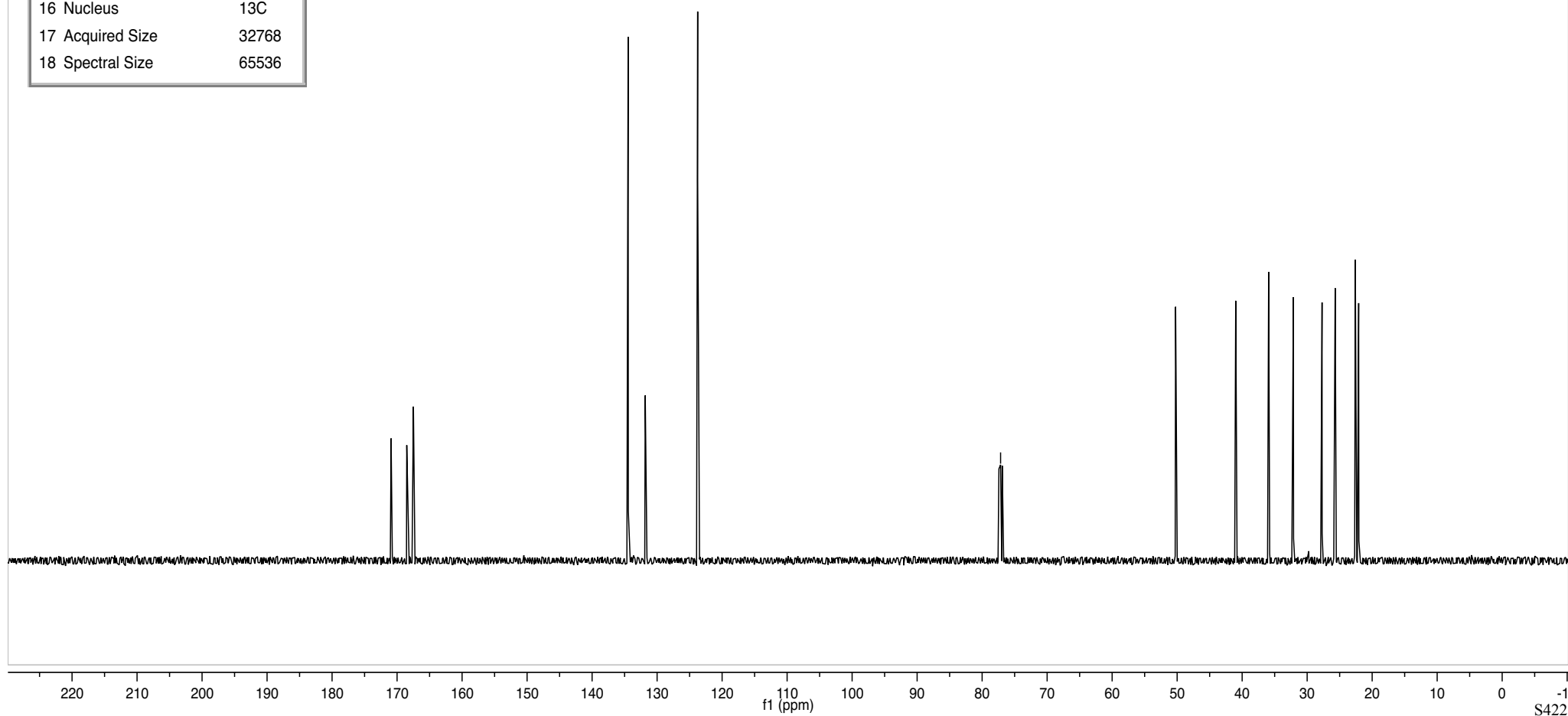
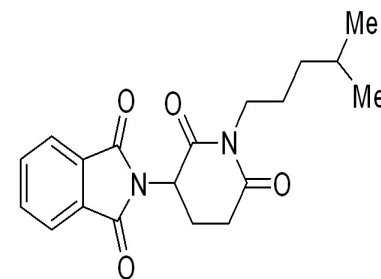
— 7.26 CDCl₃

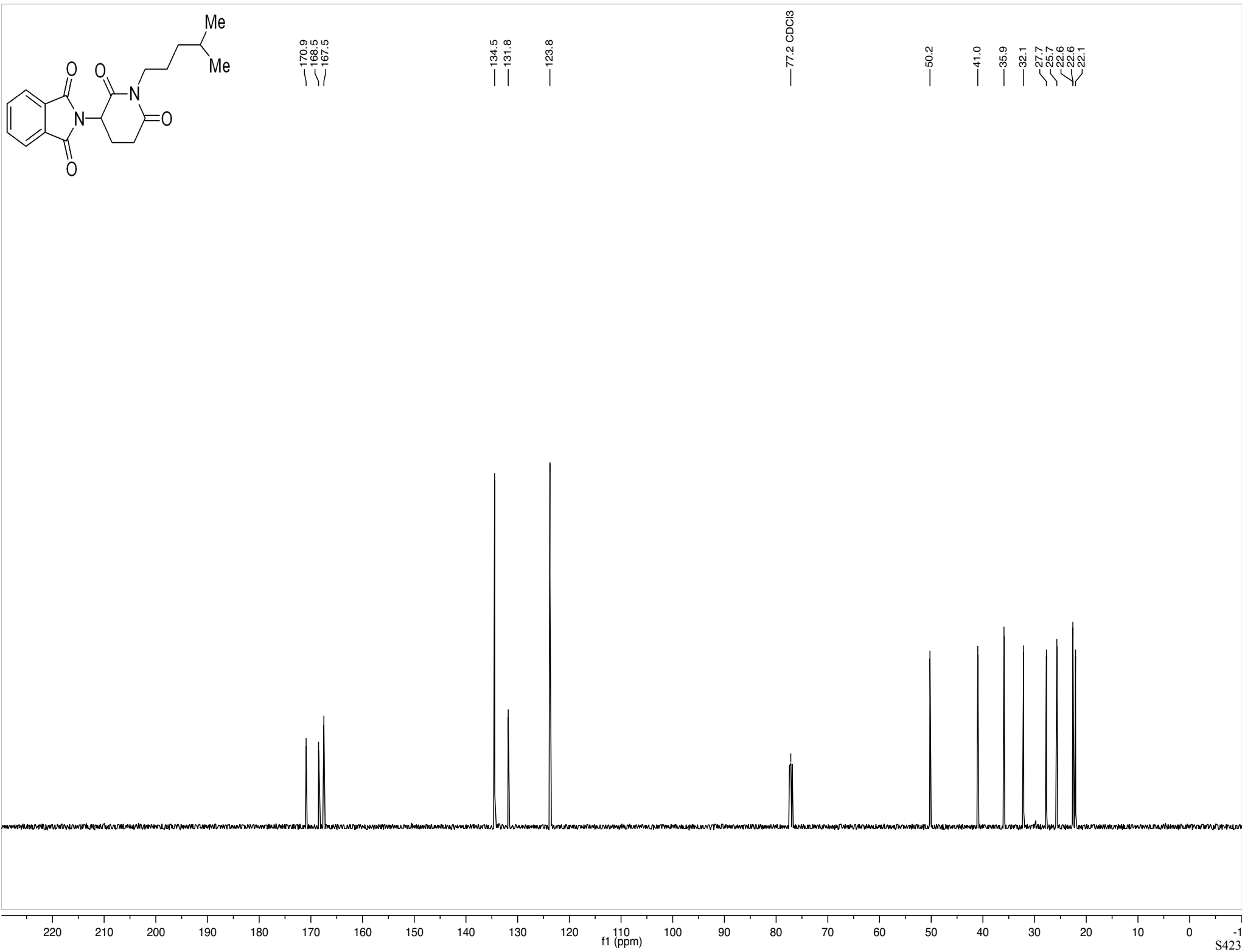




Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	96
9 Receiver Gain	60
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.0863
13 Spectrometer Frequency	125.66
14 Spectral Width	30165.9
15 Lowest Frequency	-1281.2
16 Nucleus	¹³ C
17 Acquired Size	32768
18 Spectral Size	65536

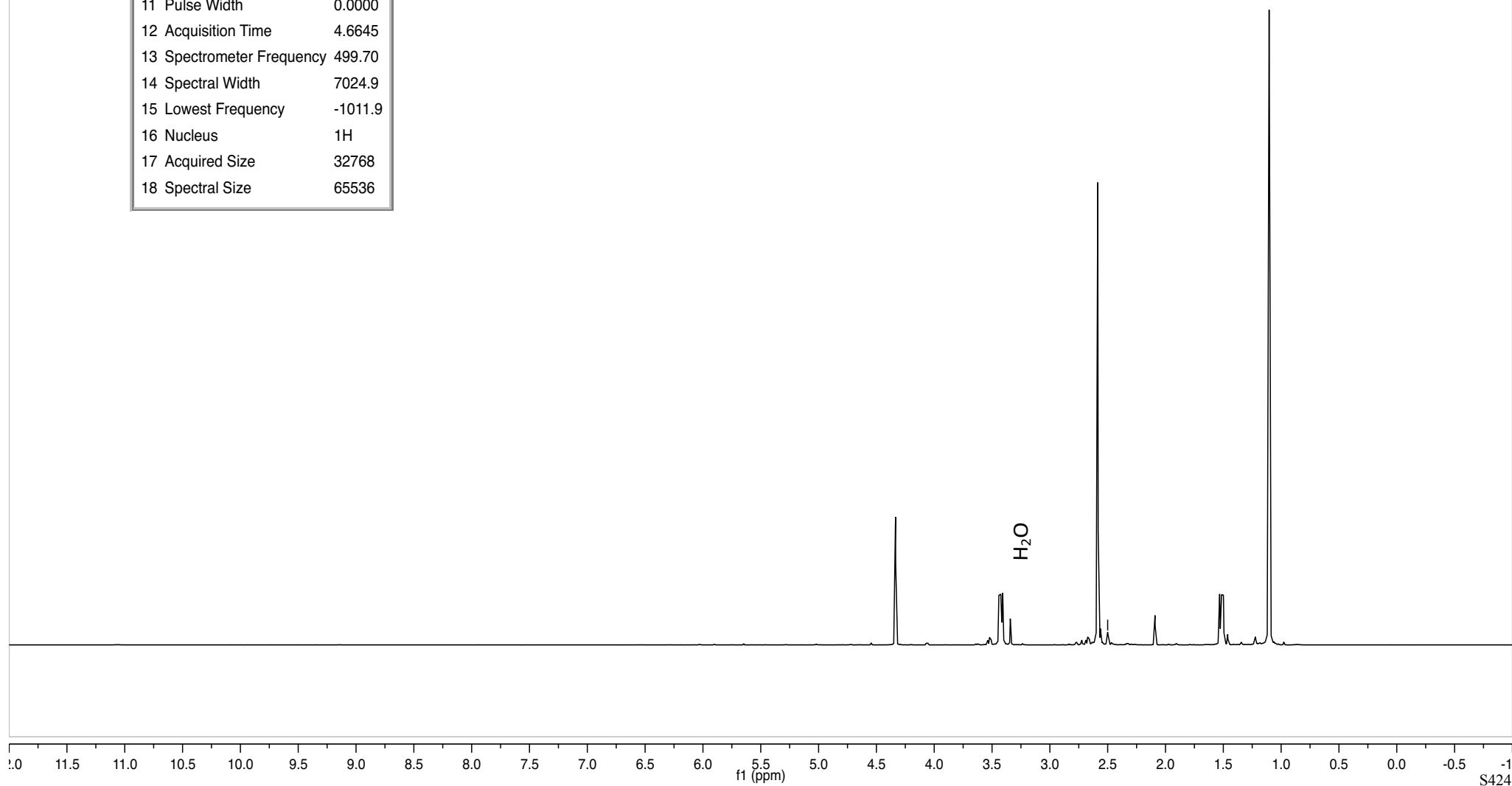
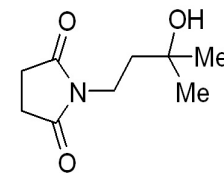
— 77.2 CDCl₃

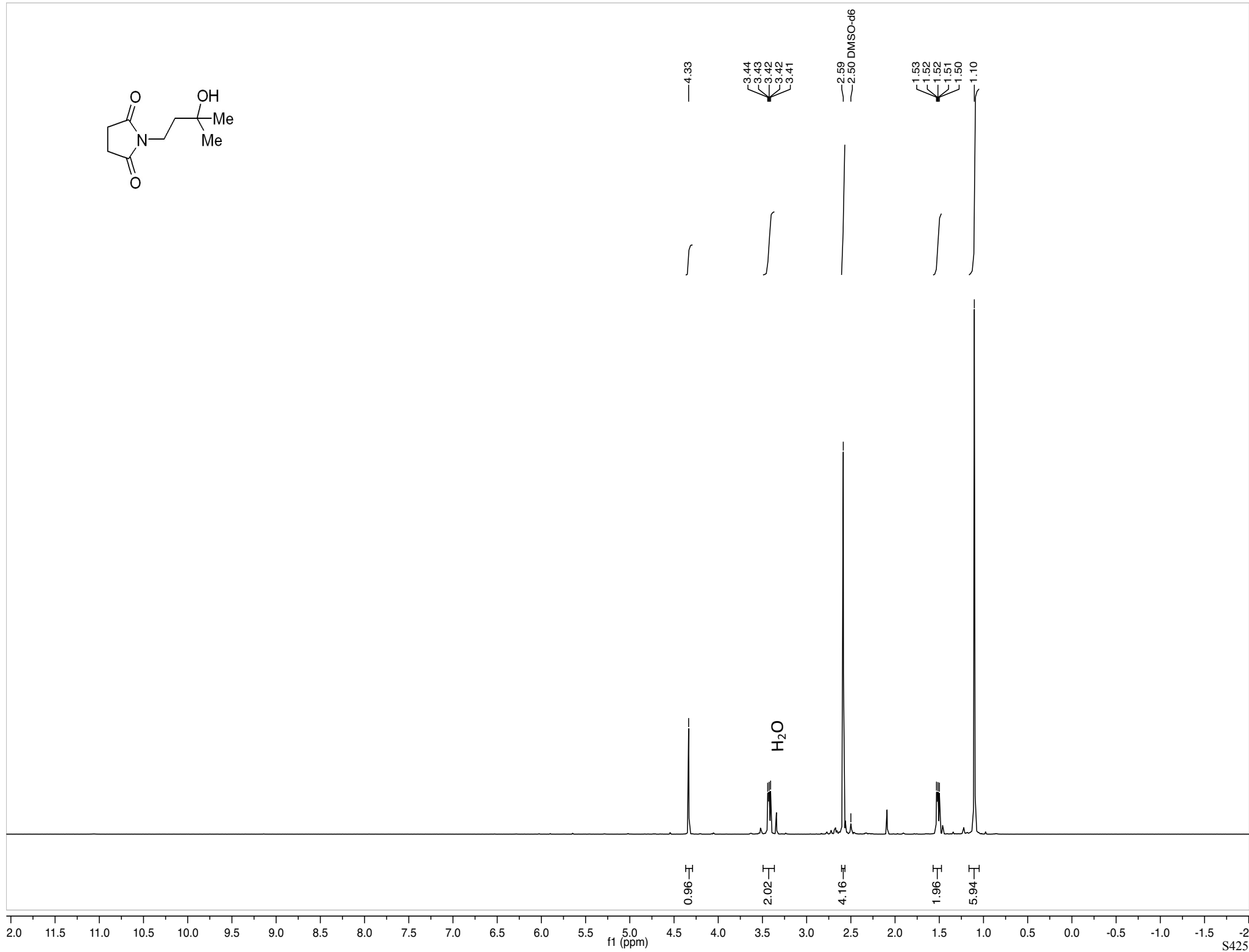
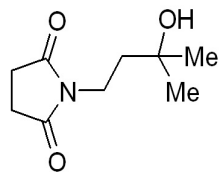




	Parameter	Value
1	Origin	Varian
2	Spectrometer	inova
3	Solvent	DMSO
4	Temperature	20.0
5	Pulse Sequence	s2pul
6	Experiment	1D
7	Probe	QUAD
8	Number of Scans	8
9	Receiver Gain	36
10	Relaxation Delay	0.0000
11	Pulse Width	0.0000
12	Acquisition Time	4.6645
13	Spectrometer Frequency	499.70
14	Spectral Width	7024.9
15	Lowest Frequency	-1011.9
16	Nucleus	^1H
17	Acquired Size	32768
18	Spectral Size	65536

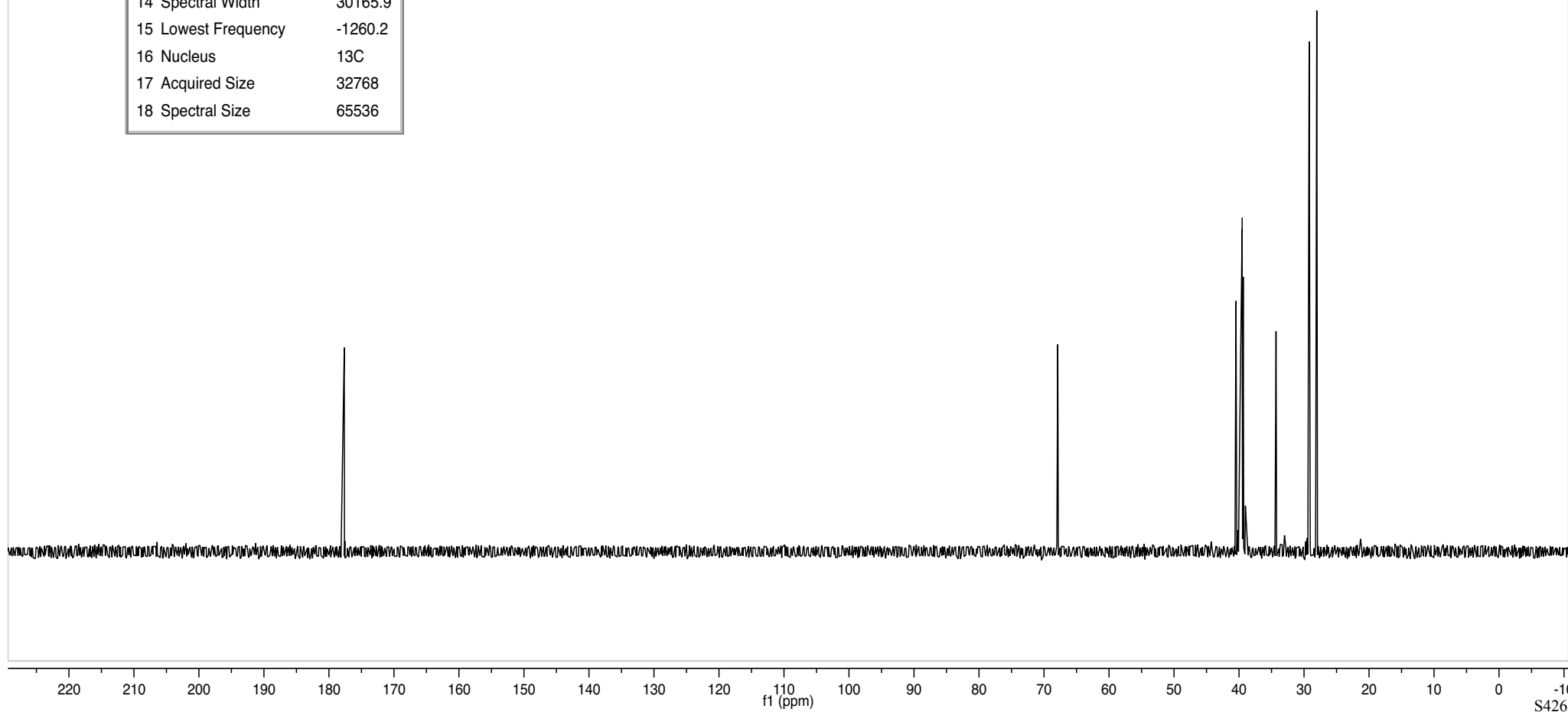
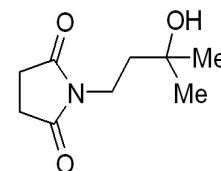
— 2.50 DMSO-d6

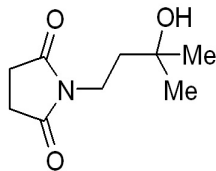




	Parameter	Value
1	Origin	Varian
2	Spectrometer	inova
3	Solvent	DMSO
4	Temperature	20.0
5	Pulse Sequence	s2pul
6	Experiment	1D
7	Probe	QUAD
8	Number of Scans	64
9	Receiver Gain	60
10	Relaxation Delay	1.0000
11	Pulse Width	0.0000
12	Acquisition Time	1.0863
13	Spectrometer Frequency	125.66
14	Spectral Width	30165.9
15	Lowest Frequency	-1260.2
16	Nucleus	¹³ C
17	Acquired Size	32768
18	Spectral Size	65536

— 39.52 DMSO-d6





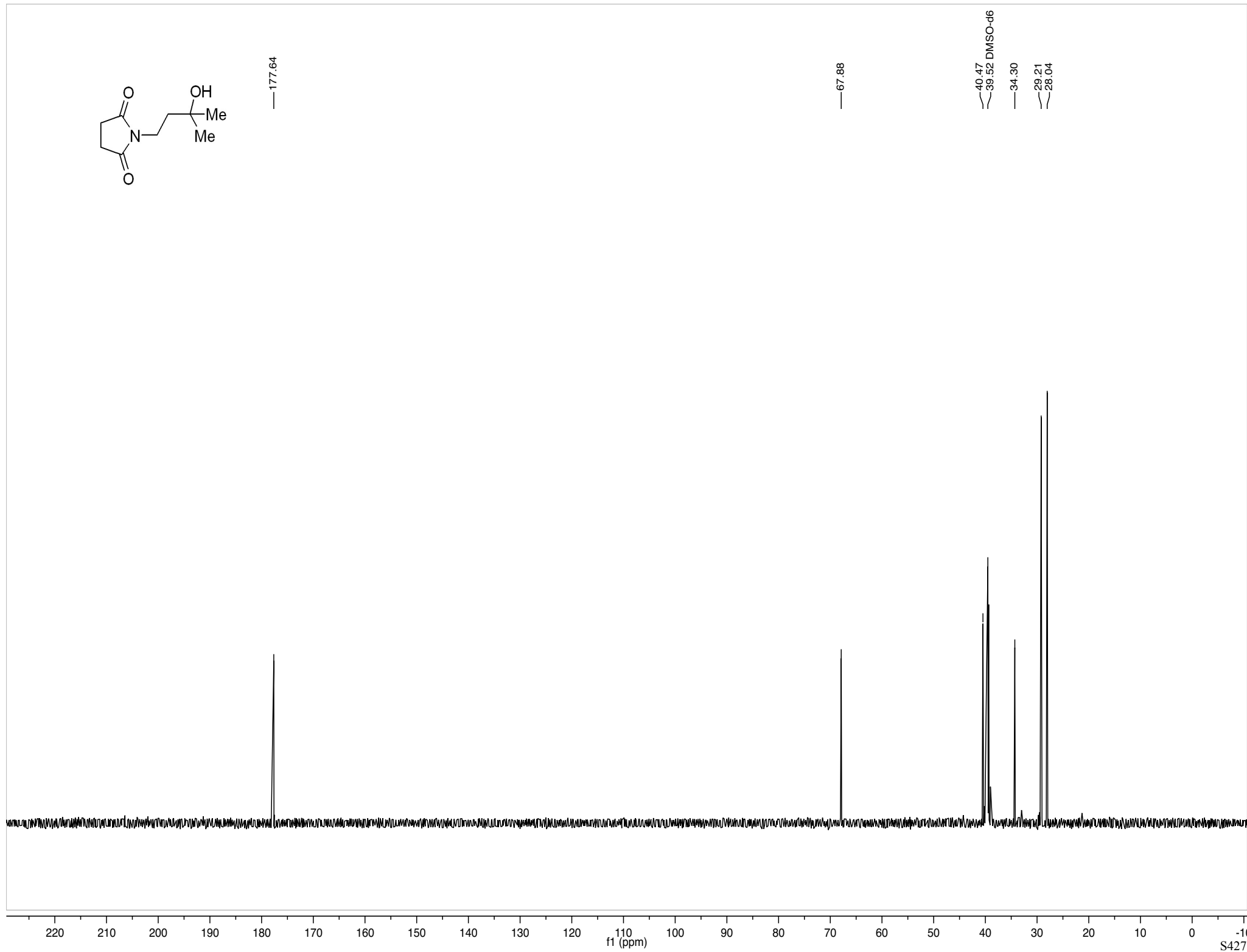
—177.64

—67.88

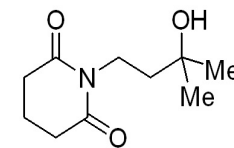
40.47
39.52 DMSO-d6

—34.30

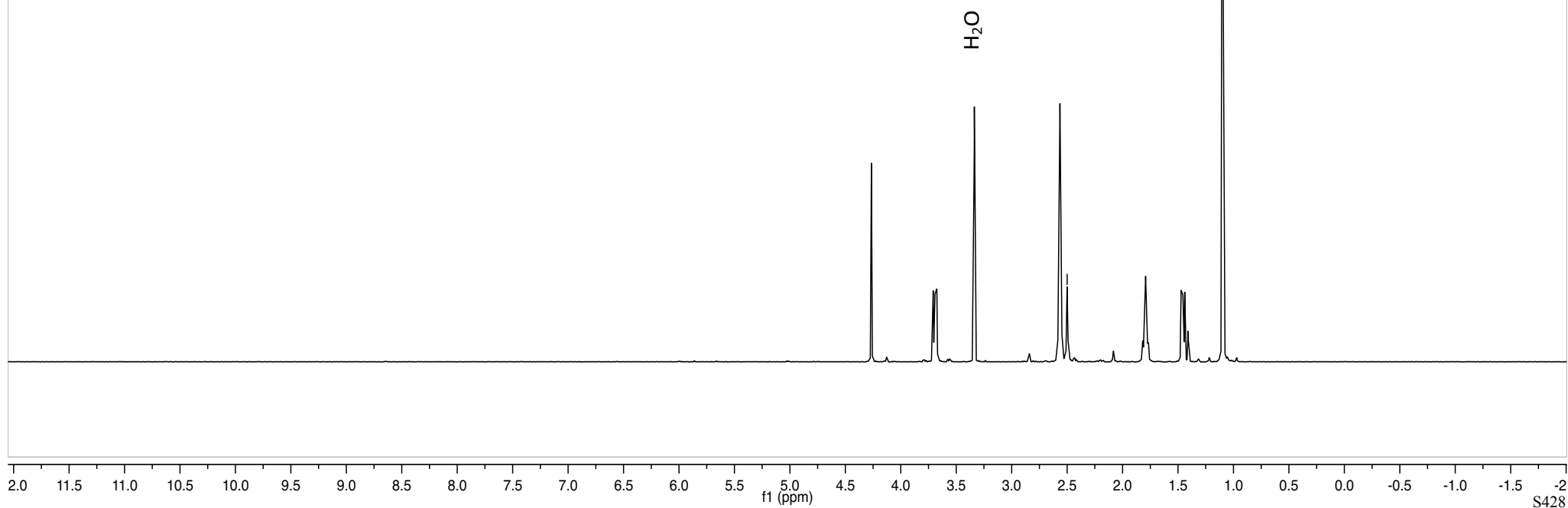
29.21
28.04

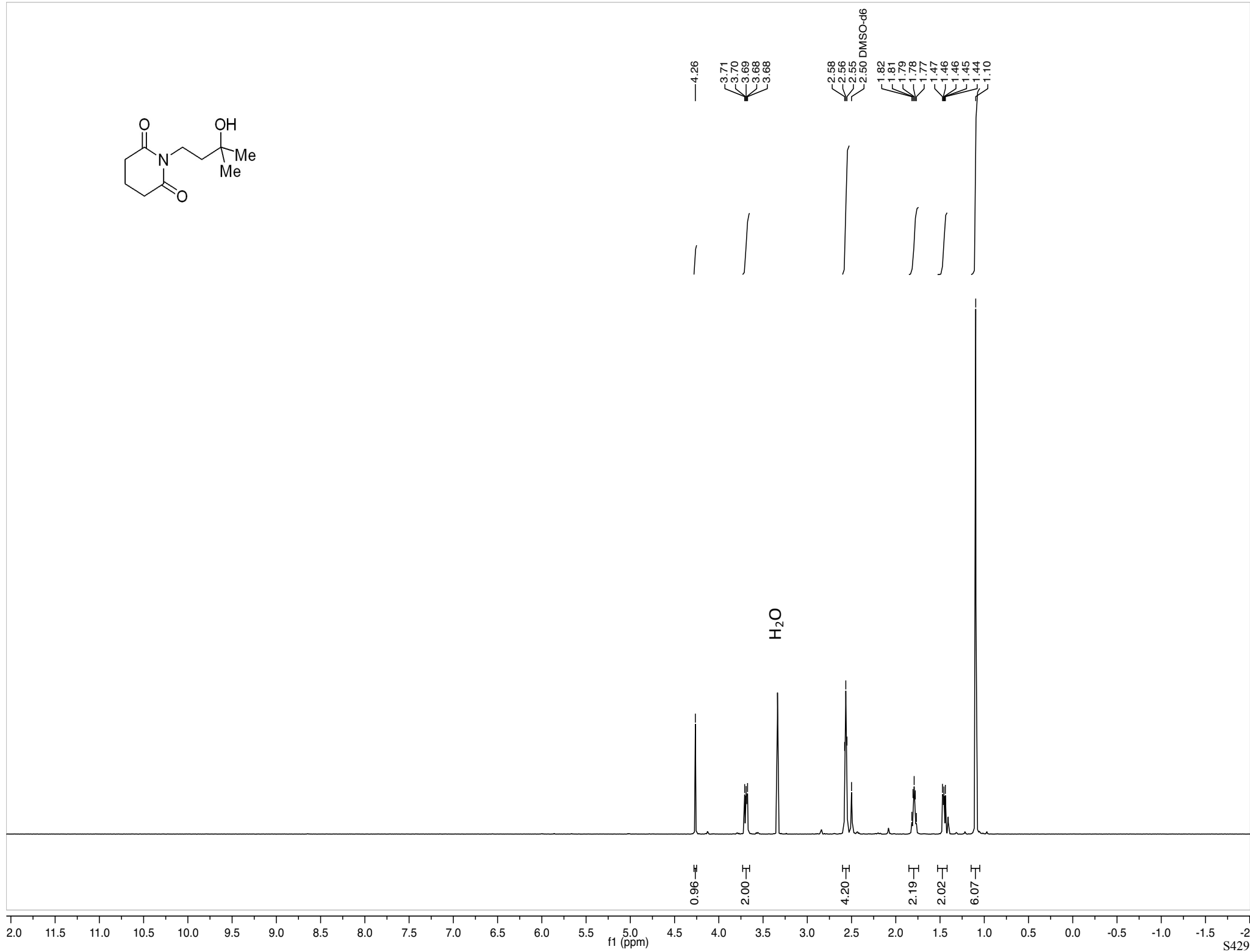
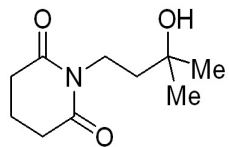


	Parameter	Value
1	Origin	Varian
2	Spectrometer	inova
3	Solvent	DMSO
4	Temperature	20.0
5	Pulse Sequence	s2pul
6	Experiment	1D
7	Probe	QUAD
8	Number of Scans	8
9	Receiver Gain	46
10	Relaxation Delay	0.0000
11	Pulse Width	0.0000
12	Acquisition Time	4.6645
13	Spectrometer Frequency	499.70
14	Spectral Width	7024.9
15	Lowest Frequency	-1002.9
16	Nucleus	¹ H
17	Acquired Size	32768
18	Spectral Size	65536



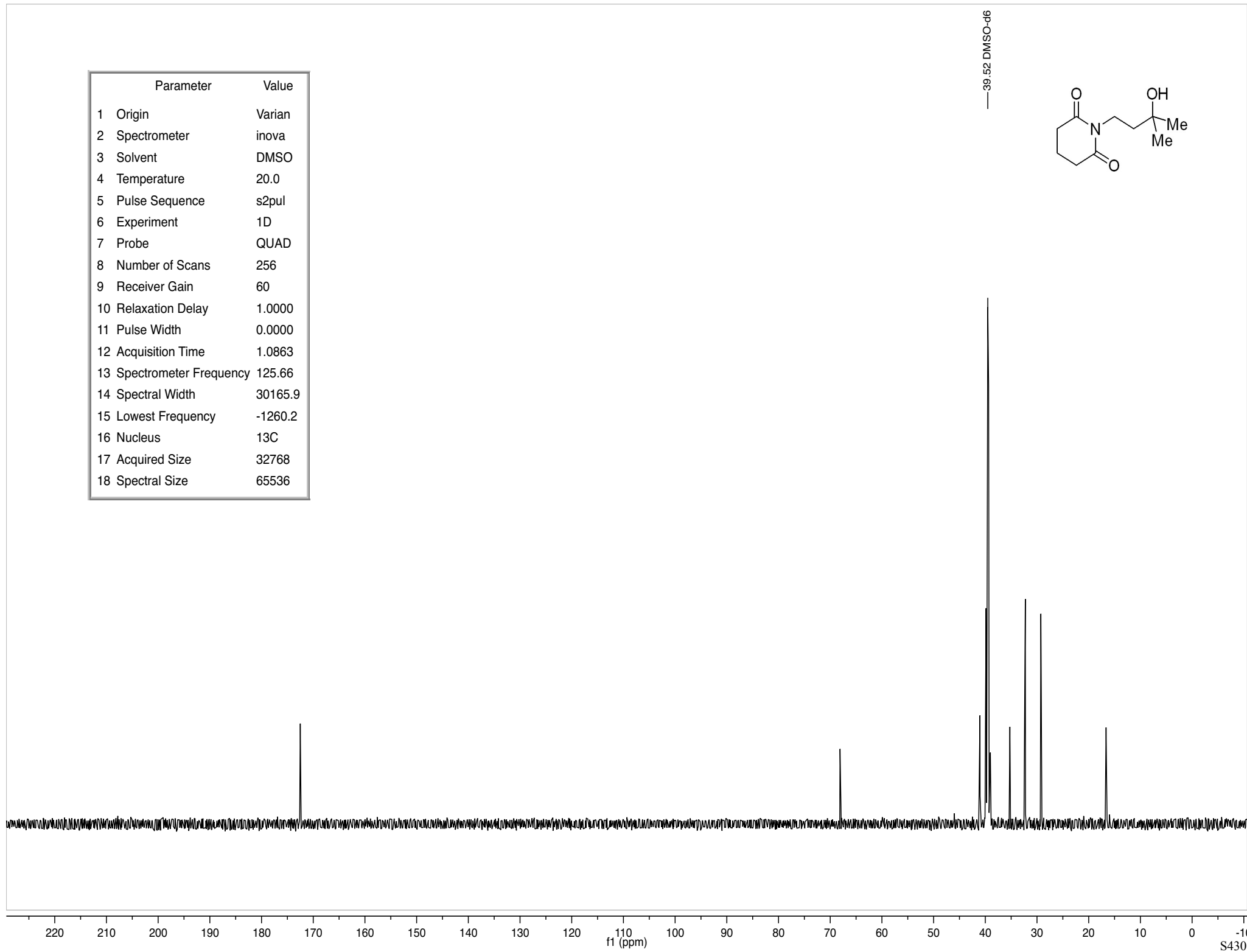
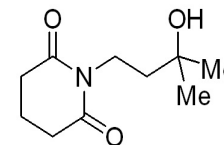
— 2.50 DMSO-d₆

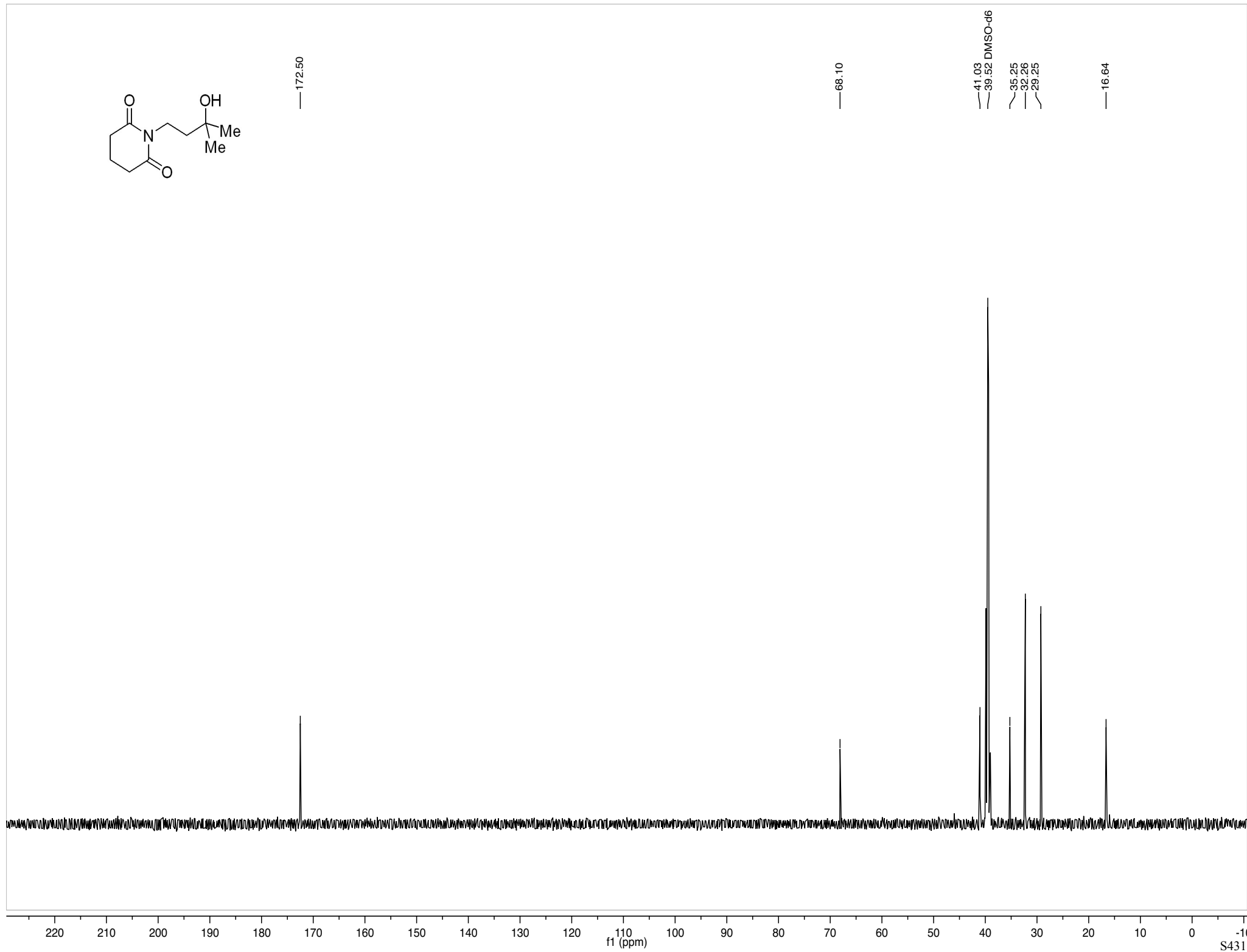
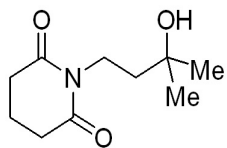




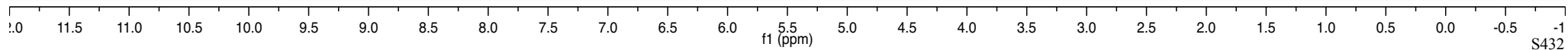
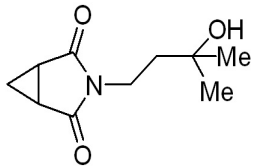
	Parameter	Value
1	Origin	Varian
2	Spectrometer	inova
3	Solvent	DMSO
4	Temperature	20.0
5	Pulse Sequence	s2pul
6	Experiment	1D
7	Probe	QUAD
8	Number of Scans	256
9	Receiver Gain	60
10	Relaxation Delay	1.0000
11	Pulse Width	0.0000
12	Acquisition Time	1.0863
13	Spectrometer Frequency	125.66
14	Spectral Width	30165.9
15	Lowest Frequency	-1260.2
16	Nucleus	¹³ C
17	Acquired Size	32768
18	Spectral Size	65536

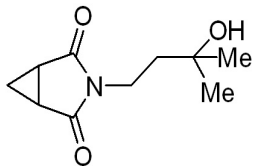
—39.52 DMSO-d6



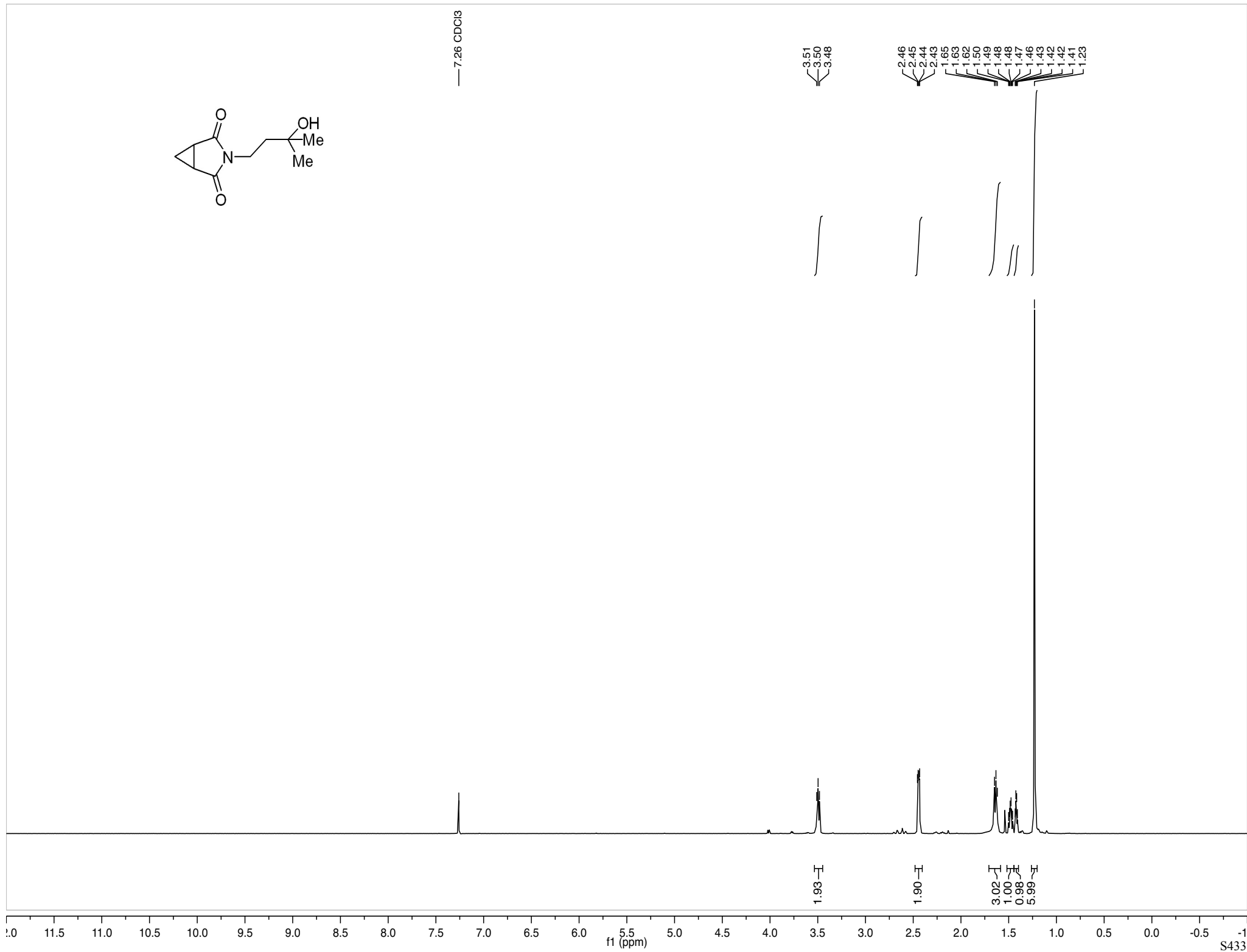


	Parameter	Value
1	Origin	Varian
2	Spectrometer	inova
3	Solvent	CDCl ₃
4	Temperature	40.0
5	Pulse Sequence	s2pul
6	Experiment	1D
7	Probe	QUAD
8	Number of Scans	8
9	Receiver Gain	46
10	Relaxation Delay	0.0000
11	Pulse Width	0.0000
12	Acquisition Time	4.6645
13	Spectrometer Frequency	499.69
14	Spectral Width	7024.9
15	Lowest Frequency	-1011.4
16	Nucleus	¹ H
17	Acquired Size	32768
18	Spectral Size	65536

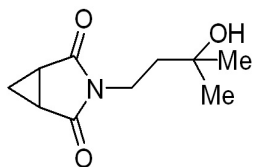
7.3 CDCl₃



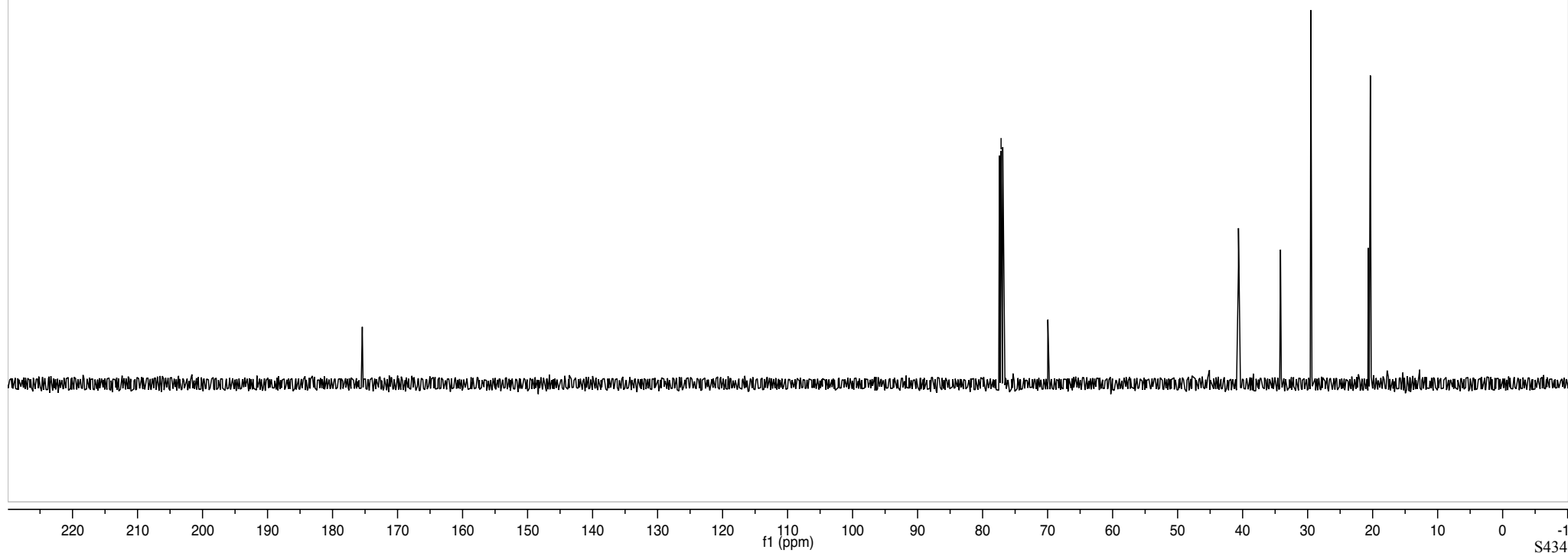
— 7.26 CDCl₃

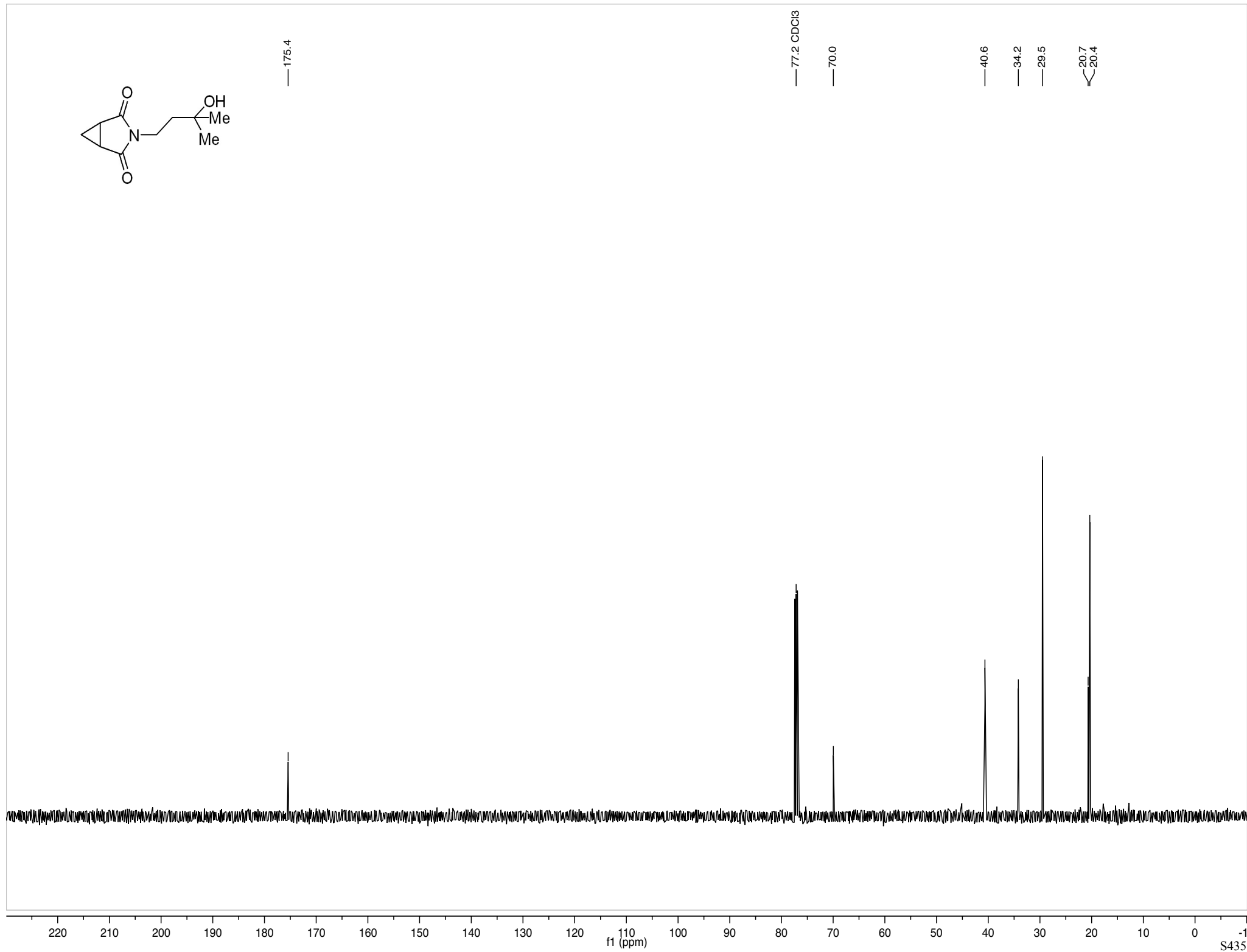
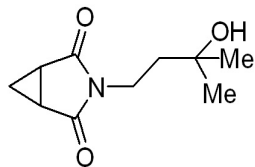


Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	40.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	192
9 Receiver Gain	60
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.0863
13 Spectrometer Frequency	125.66
14 Spectral Width	30165.9
15 Lowest Frequency	-1271.8
16 Nucleus	¹³ C
17 Acquired Size	32768
18 Spectral Size	65536



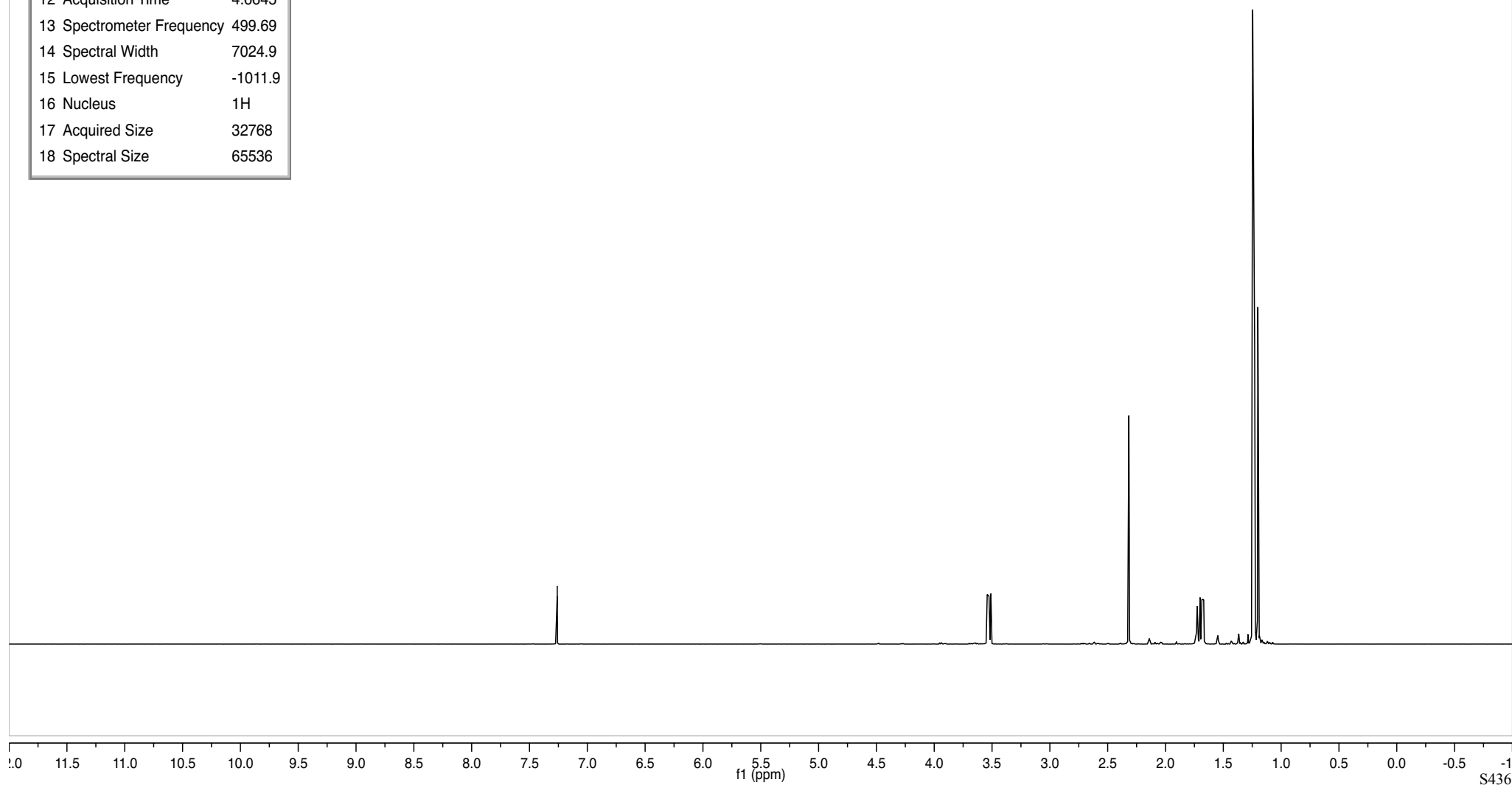
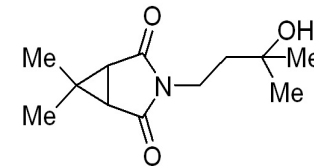
— 77.2 CDCl₃

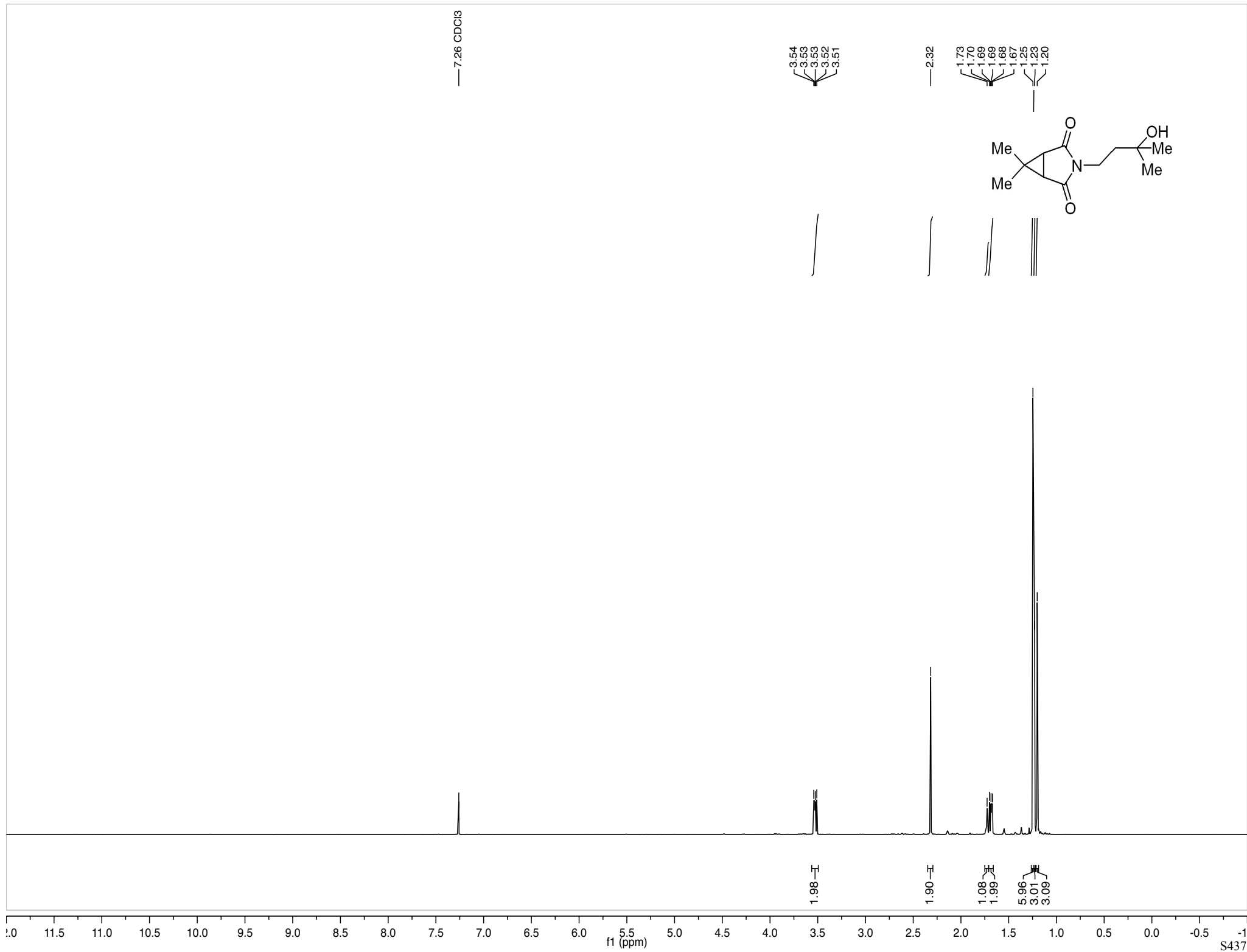




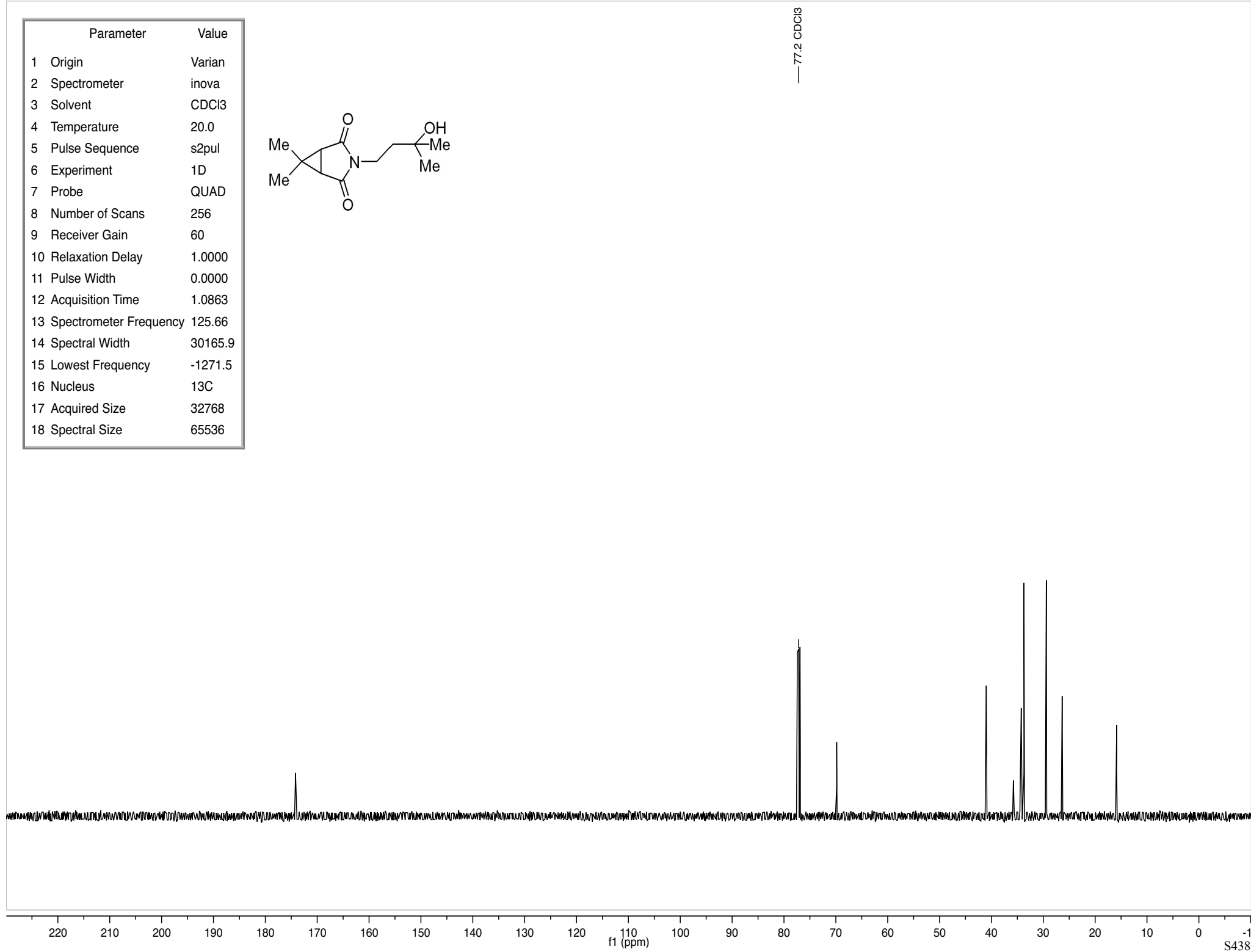
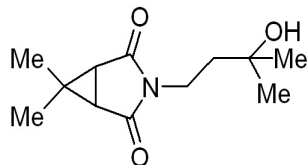
Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	8
9 Receiver Gain	46
10 Relaxation Delay	0.0000
11 Pulse Width	0.0000
12 Acquisition Time	4.6645
13 Spectrometer Frequency	499.69
14 Spectral Width	7024.9
15 Lowest Frequency	-1011.9
16 Nucleus	¹ H
17 Acquired Size	32768
18 Spectral Size	65536

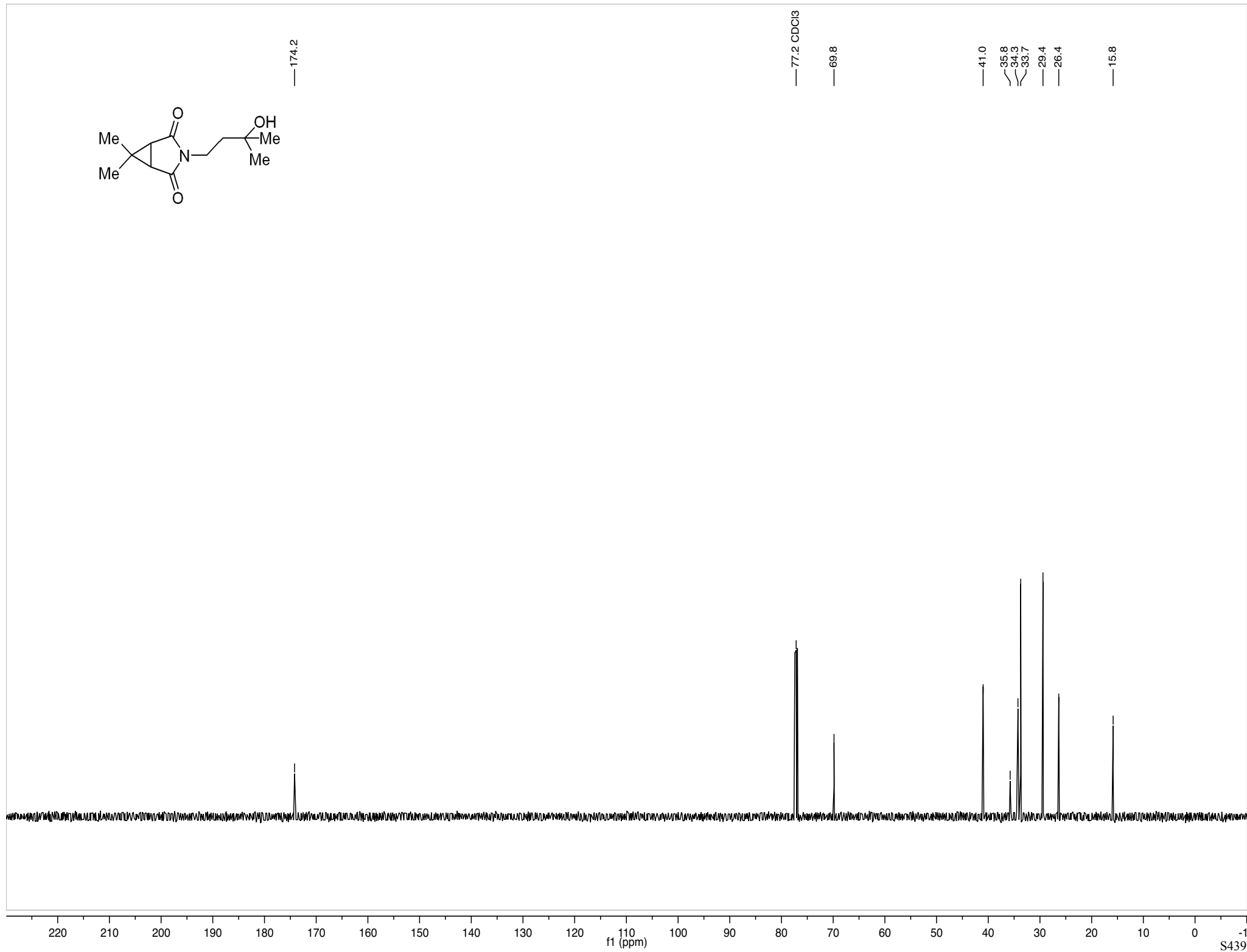
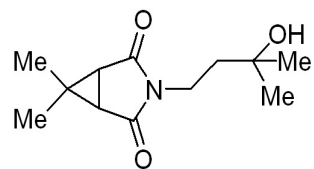
—7.3 CDCl₃





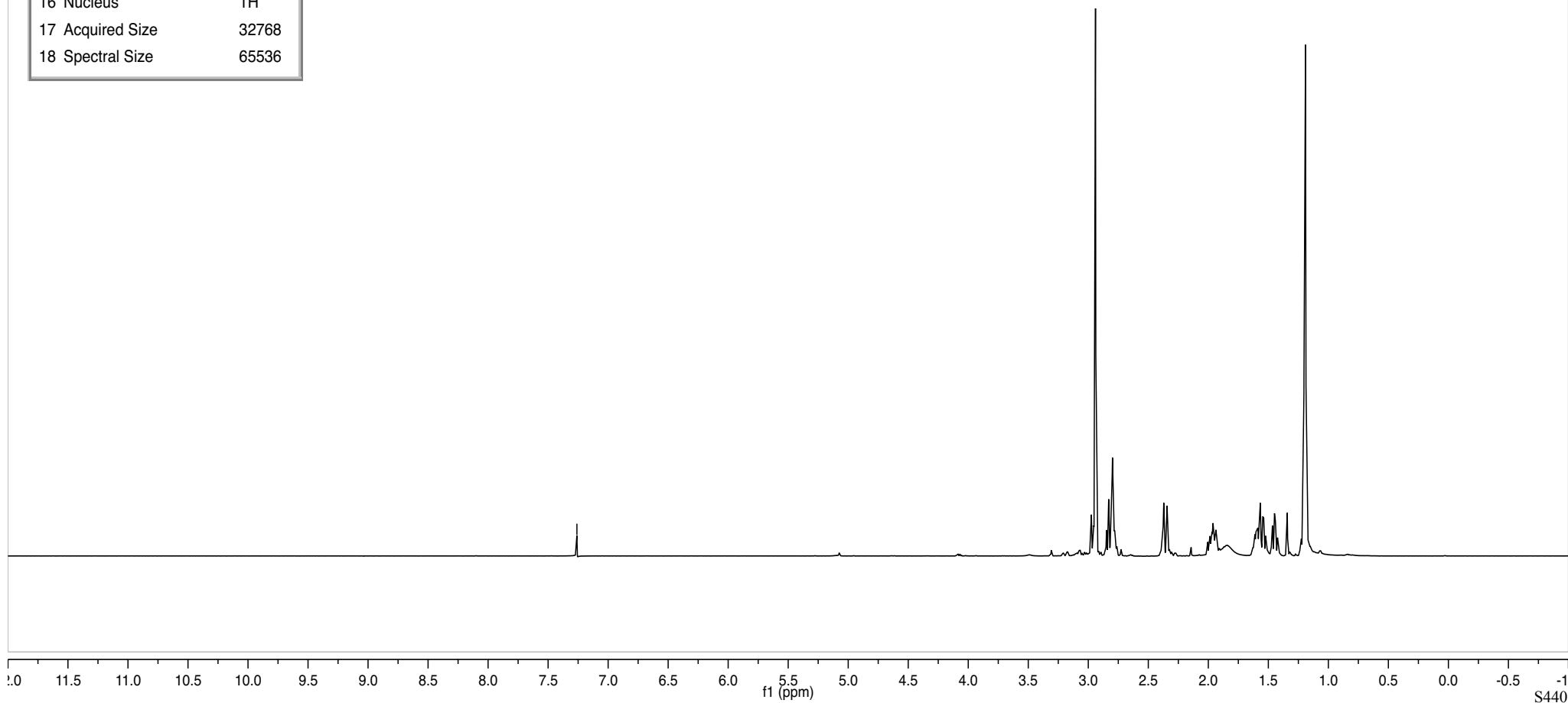
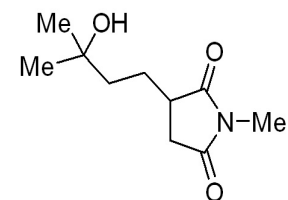
Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	256
9 Receiver Gain	60
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.0863
13 Spectrometer Frequency	125.66
14 Spectral Width	30165.9
15 Lowest Frequency	-1271.5
16 Nucleus	¹³ C
17 Acquired Size	32768
18 Spectral Size	65536

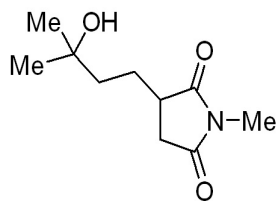




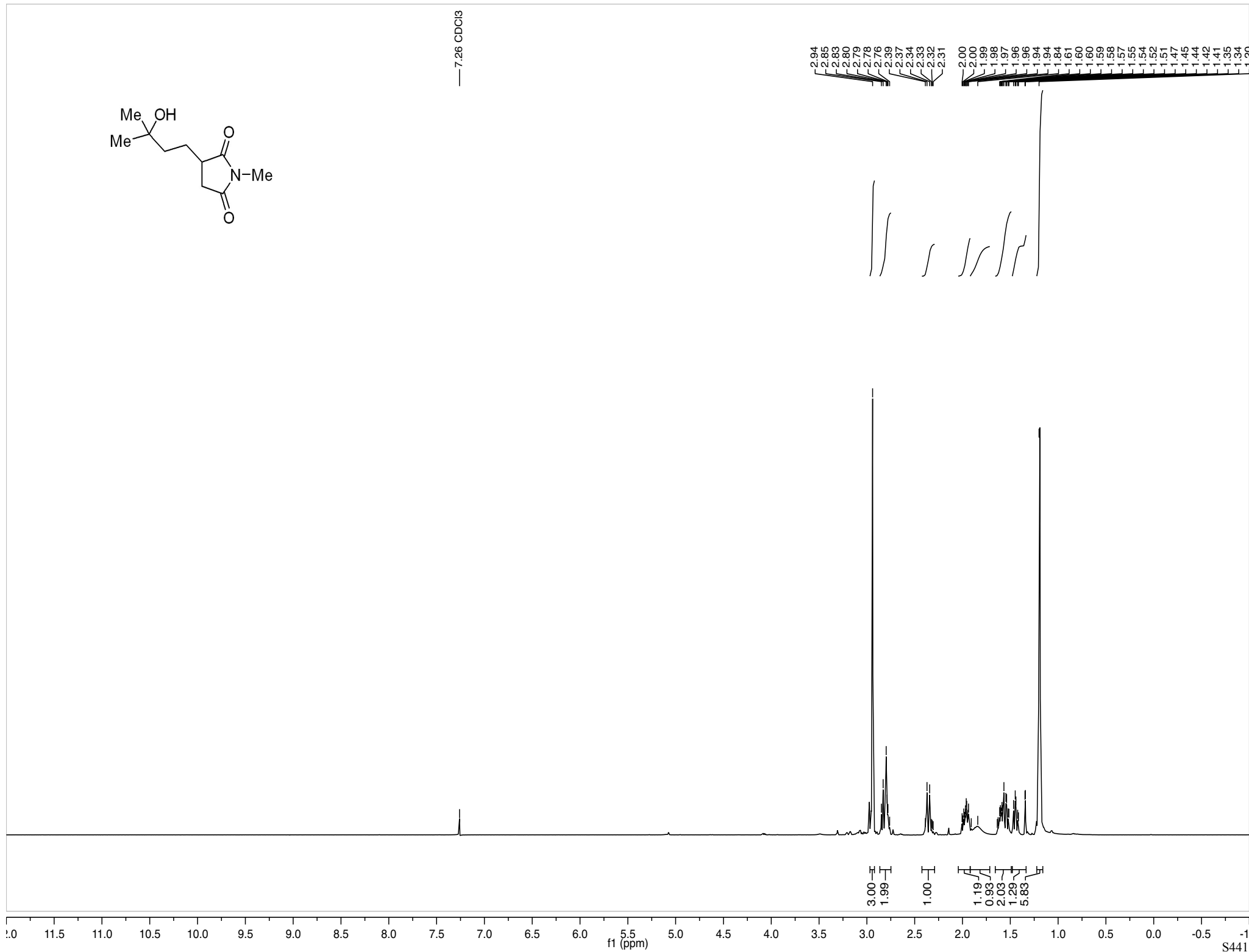
	Parameter	Value
1	Origin	Varian
2	Spectrometer	inova
3	Solvent	CDCl3
4	Temperature	20.0
5	Pulse Sequence	s2pul
6	Experiment	1D
7	Probe	QUAD
8	Number of Scans	8
9	Receiver Gain	36
10	Relaxation Delay	0.0000
11	Pulse Width	0.0000
12	Acquisition Time	4.6645
13	Spectrometer Frequency	499.69
14	Spectral Width	7024.9
15	Lowest Frequency	-1020.9
16	Nucleus	¹ H
17	Acquired Size	32768
18	Spectral Size	65536

— 7.3 CDCl₃

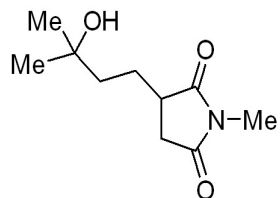




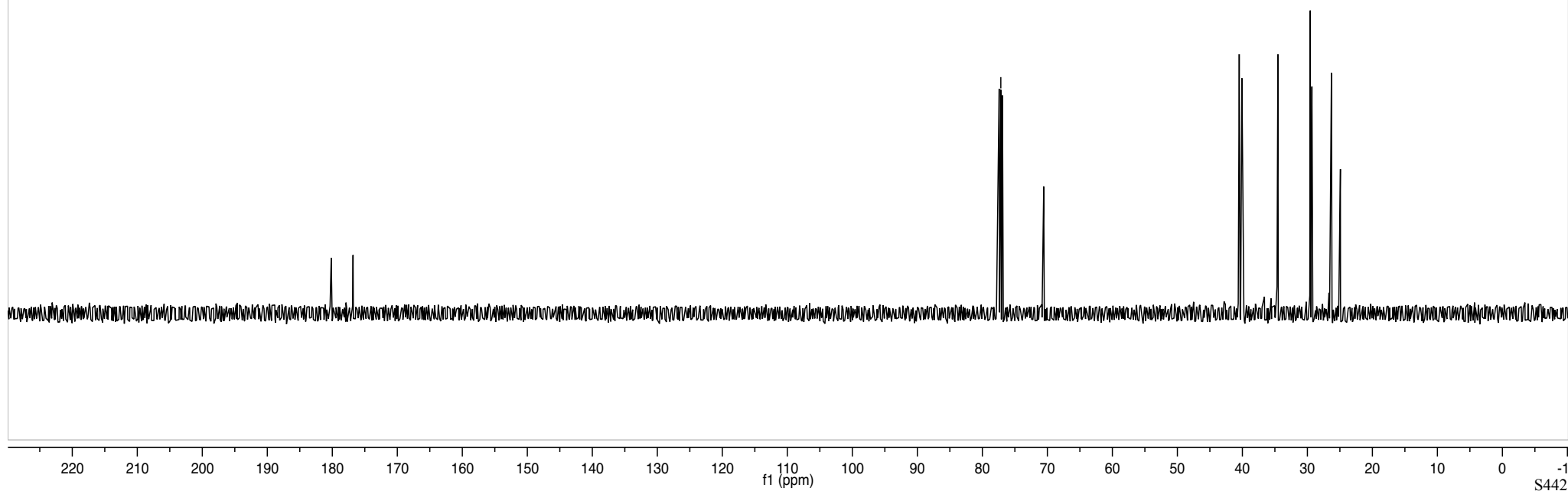
— 7.26 CDCl₃

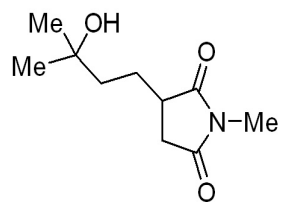


Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	112
9 Receiver Gain	60
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.0863
13 Spectrometer Frequency	125.66
14 Spectral Width	30165.9
15 Lowest Frequency	-1276.6
16 Nucleus	13C
17 Acquired Size	32768
18 Spectral Size	65536



— 77.2 CDCl3





— 180.2
— 176.8

— 77.2 CDCl₃

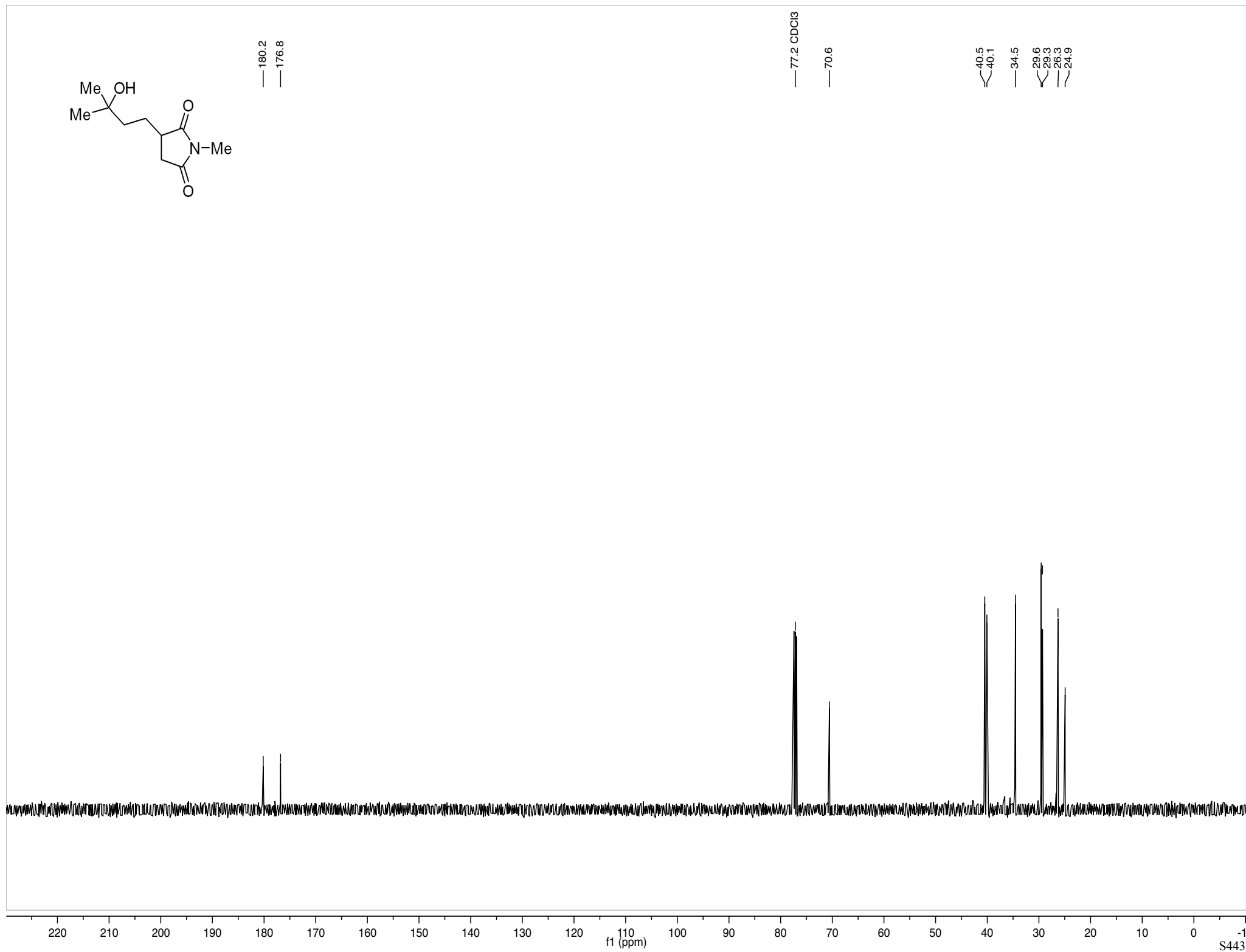
— 70.6

— 40.5
— 40.1

— 34.5

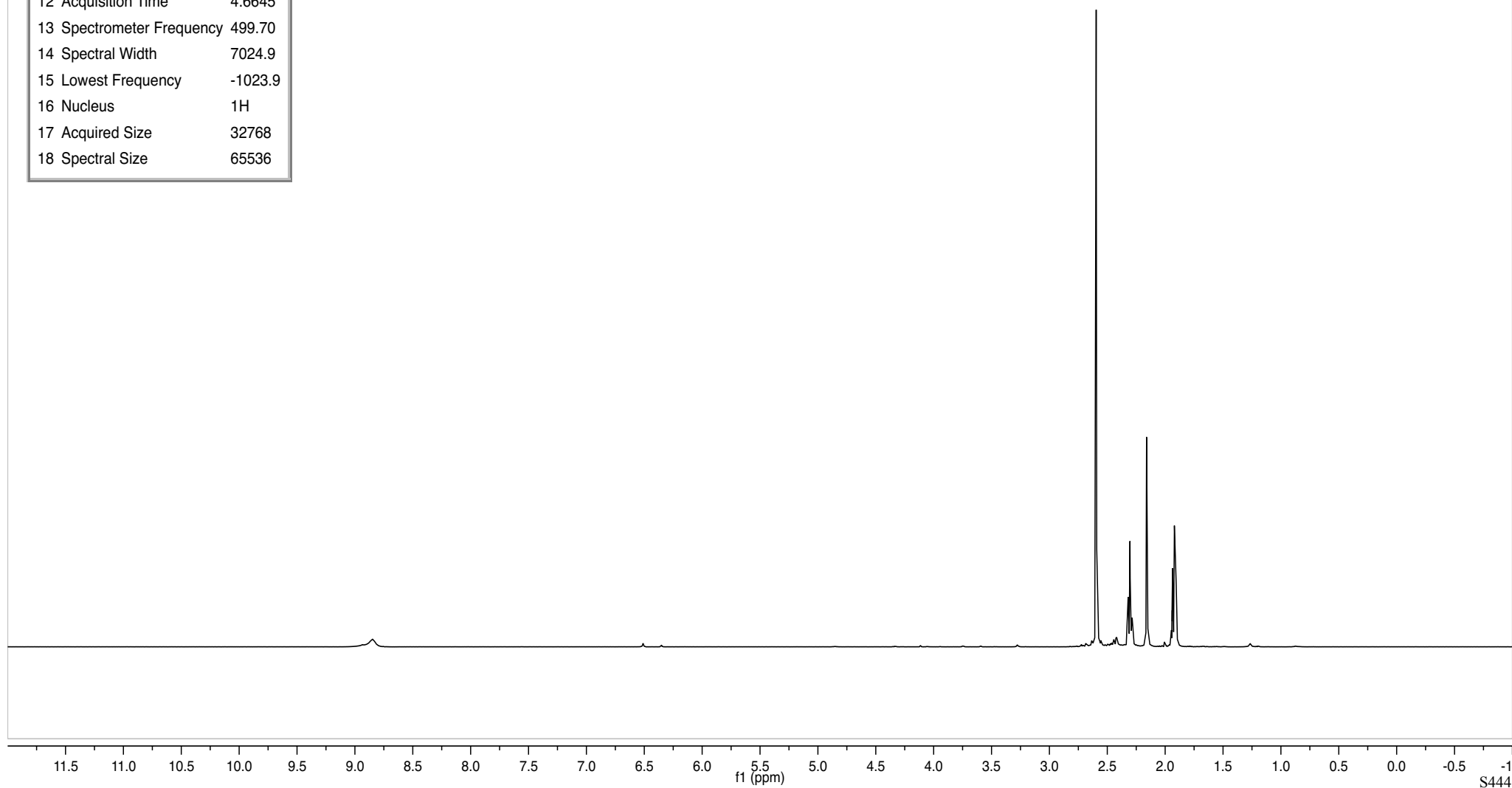
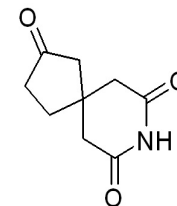
— 29.6
— 29.3

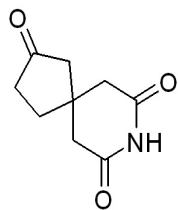
— 26.3
— 24.9



Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CD3CN
4 Temperature	29.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	8
9 Receiver Gain	41
10 Relaxation Delay	0.0000
11 Pulse Width	0.0000
12 Acquisition Time	4.6645
13 Spectrometer Frequency	499.70
14 Spectral Width	7024.9
15 Lowest Frequency	-1023.9
16 Nucleus	¹ H
17 Acquired Size	32768
18 Spectral Size	65536

— 1.94 CD3CN

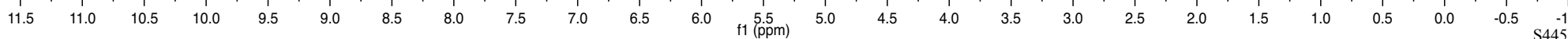




0.91

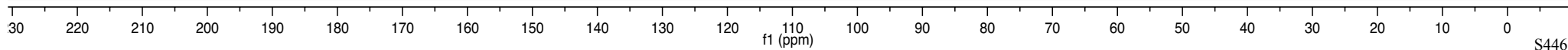
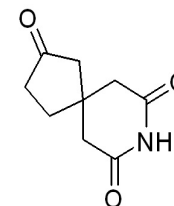
2.60
2.32
2.30
2.29
2.16
1.94 CD3CN
1.94
1.92
1.90

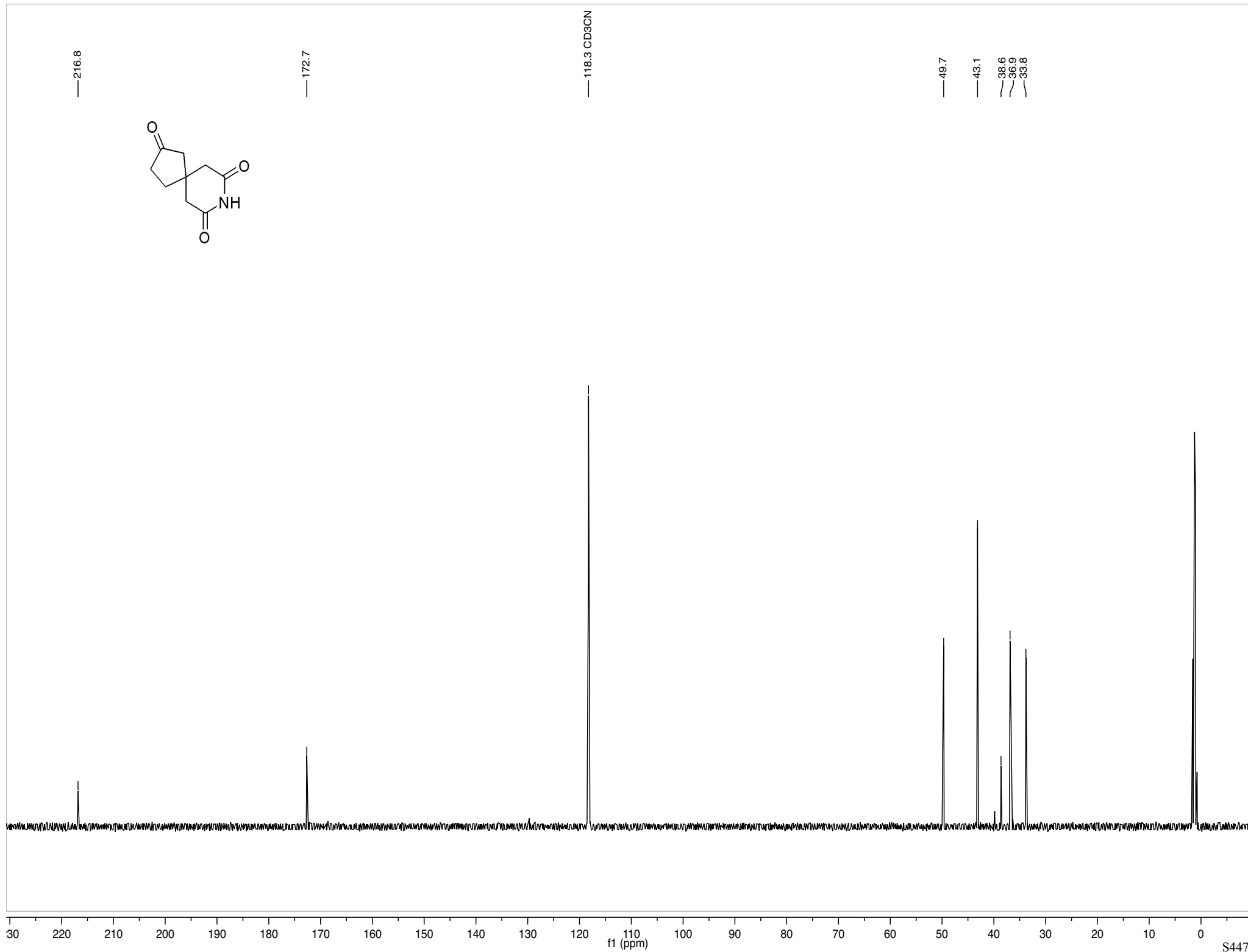
4.20
2.12
2.00
2.34

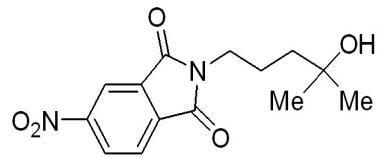


Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CD3CN
4 Temperature	22.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	240
9 Receiver Gain	60
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.0863
13 Spectrometer Frequency	125.66
14 Spectral Width	30165.9
15 Lowest Frequency	-1260.2
16 Nucleus	¹³ C
17 Acquired Size	32768
18 Spectral Size	65536

— 118.3 CD3CN

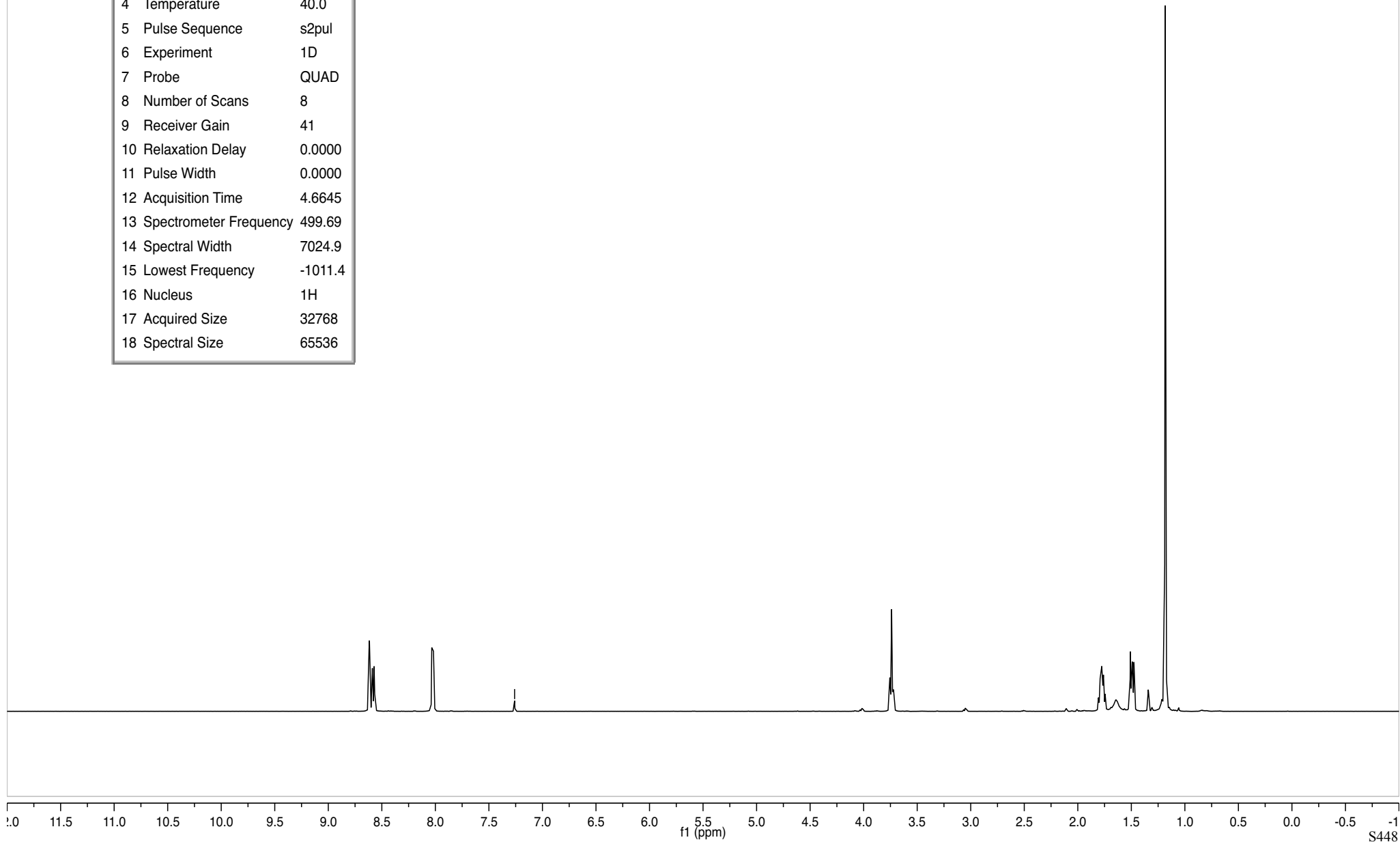


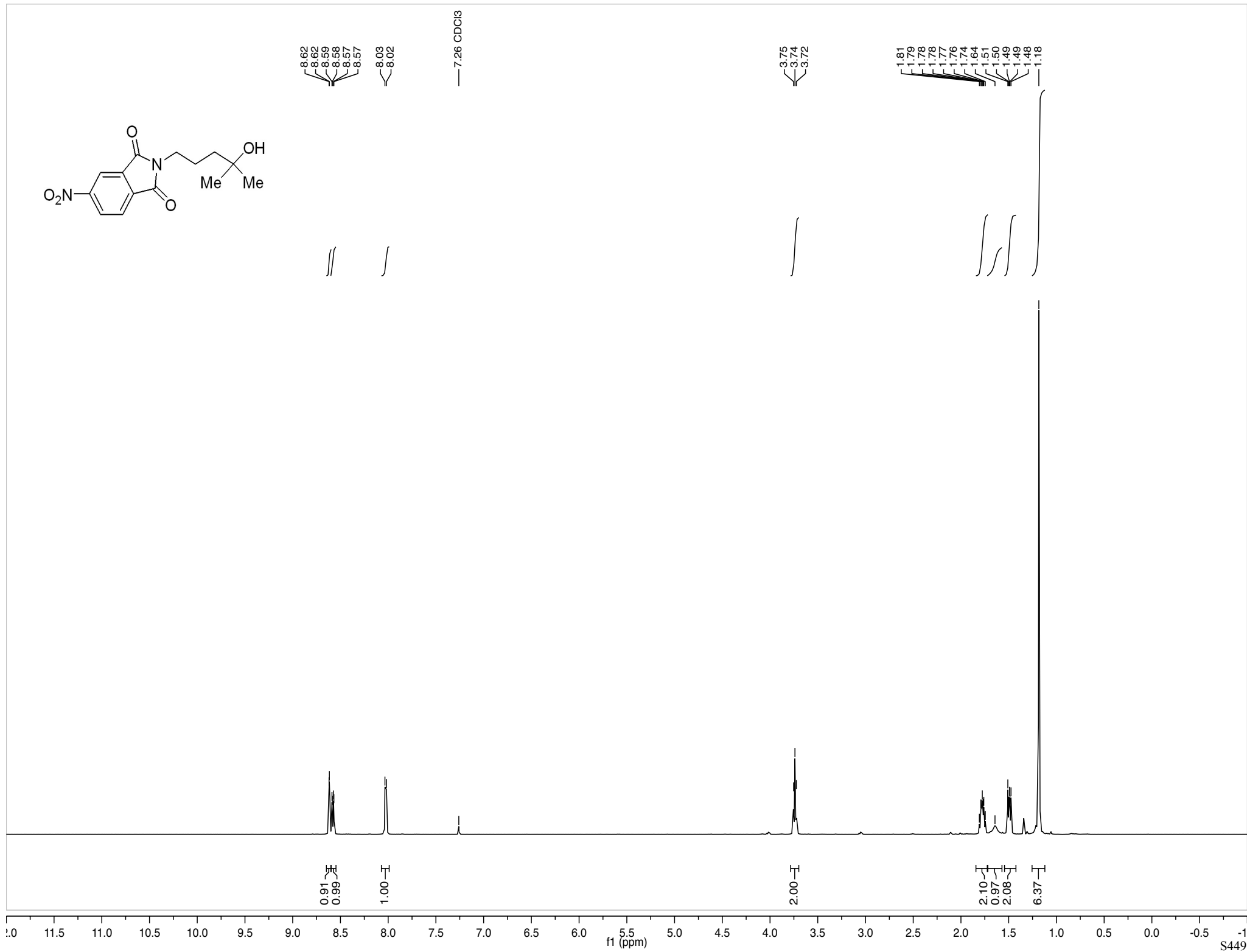
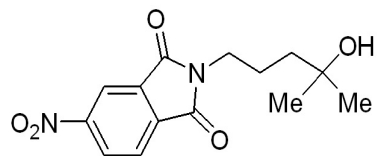




— 7.26 CDCl₃

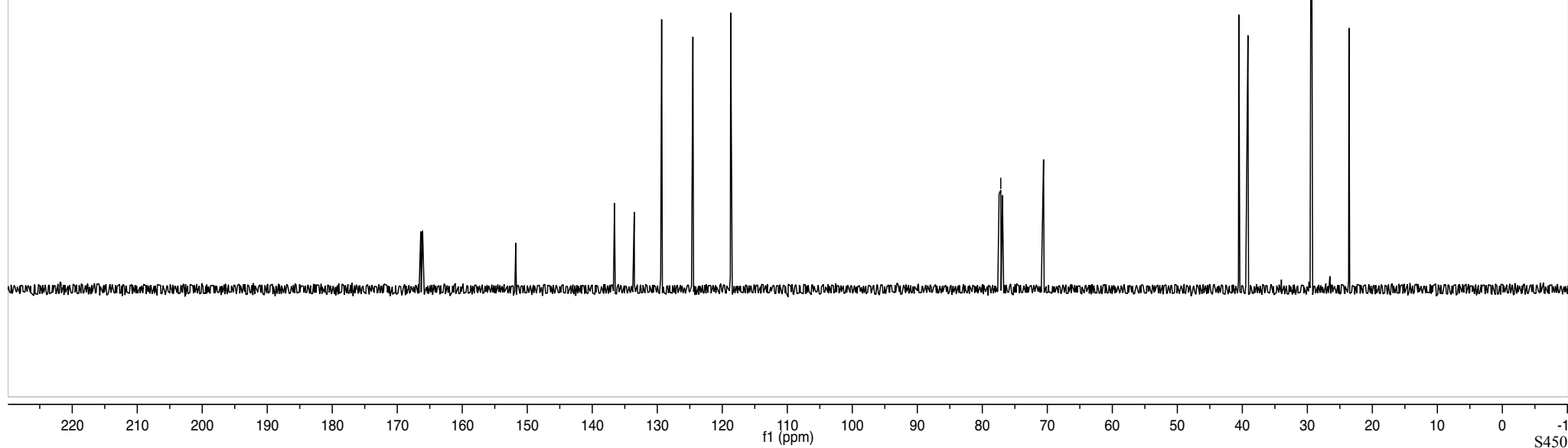
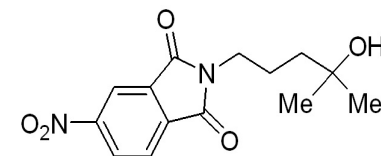
Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl ₃
4 Temperature	40.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	8
9 Receiver Gain	41
10 Relaxation Delay	0.0000
11 Pulse Width	0.0000
12 Acquisition Time	4.6645
13 Spectrometer Frequency	499.69
14 Spectral Width	7024.9
15 Lowest Frequency	-1011.4
16 Nucleus	¹ H
17 Acquired Size	32768
18 Spectral Size	65536

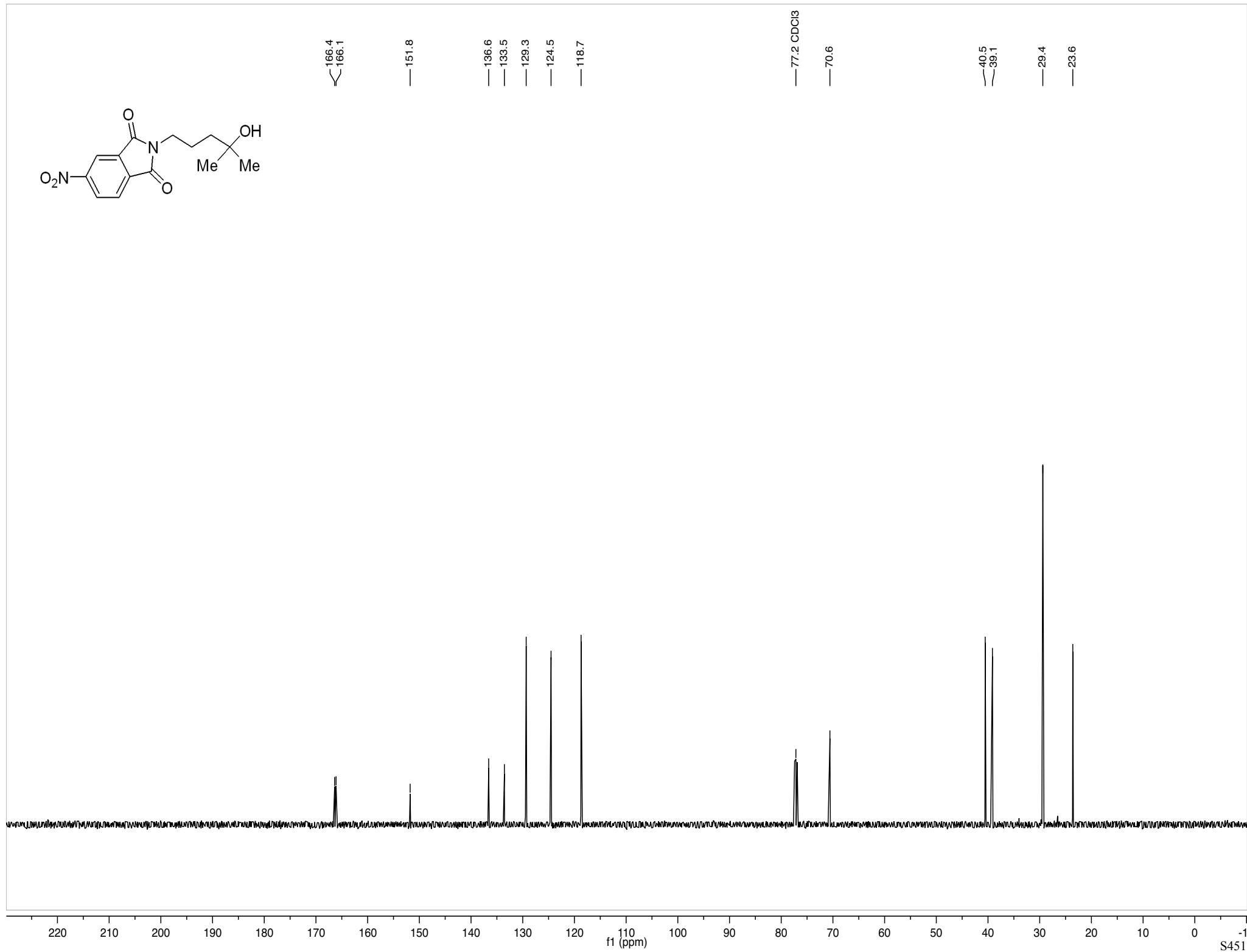
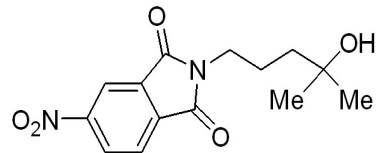


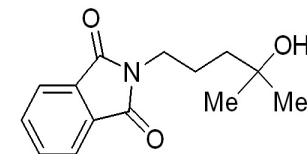


	Parameter	Value
1	Origin	Varian
2	Spectrometer	inova
3	Solvent	CDCl3
4	Temperature	40.0
5	Pulse Sequence	s2pul
6	Experiment	1D
7	Probe	QUAD
8	Number of Scans	64
9	Receiver Gain	60
10	Relaxation Delay	1.0000
11	Pulse Width	0.0000
12	Acquisition Time	1.0863
13	Spectrometer Frequency	125.66
14	Spectral Width	30165.9
15	Lowest Frequency	-1260.2
16	Nucleus	¹³ C
17	Acquired Size	32768
18	Spectral Size	65536

— 77.16 CDCl₃

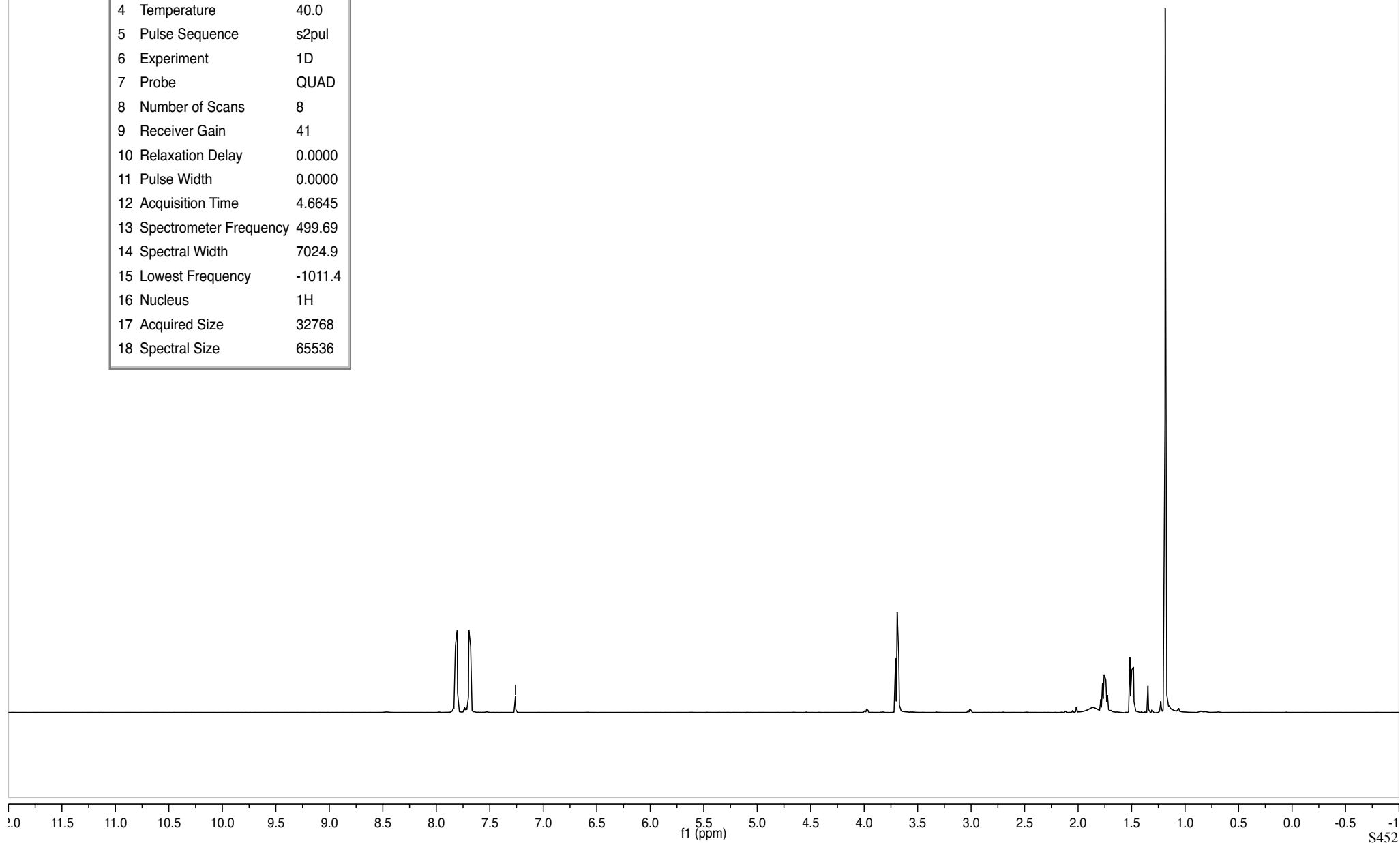


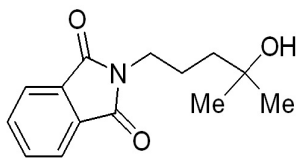




— 7.26 CDCl₃

Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl ₃
4 Temperature	40.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	8
9 Receiver Gain	41
10 Relaxation Delay	0.0000
11 Pulse Width	0.0000
12 Acquisition Time	4.6645
13 Spectrometer Frequency	499.69
14 Spectral Width	7024.9
15 Lowest Frequency	-1011.4
16 Nucleus	¹ H
17 Acquired Size	32768
18 Spectral Size	65536

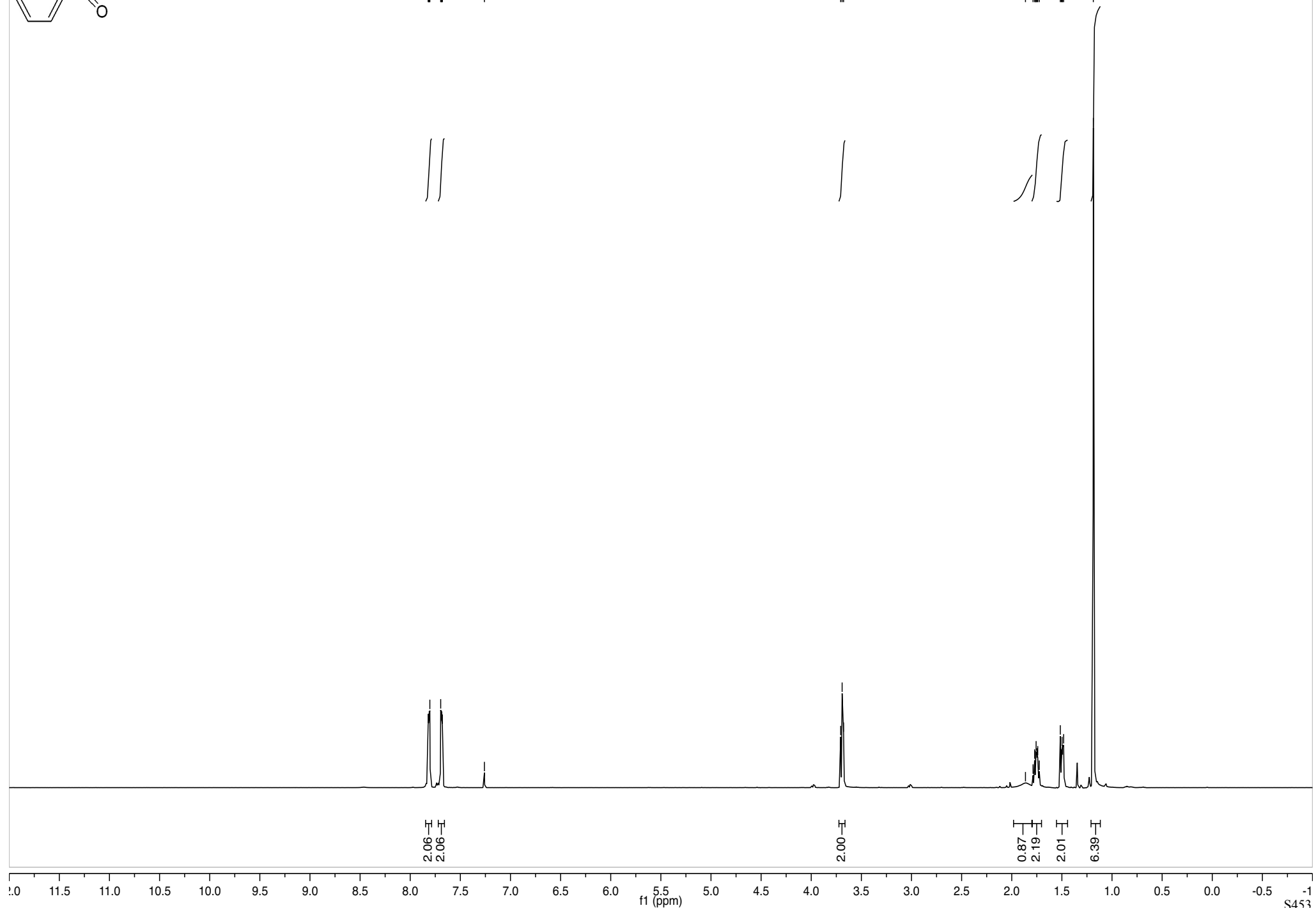


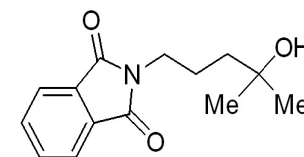


7.82
7.81
7.81
7.80
7.70
7.69
7.69
7.68
— 7.26 CDCl₃

3.71
3.69
3.68

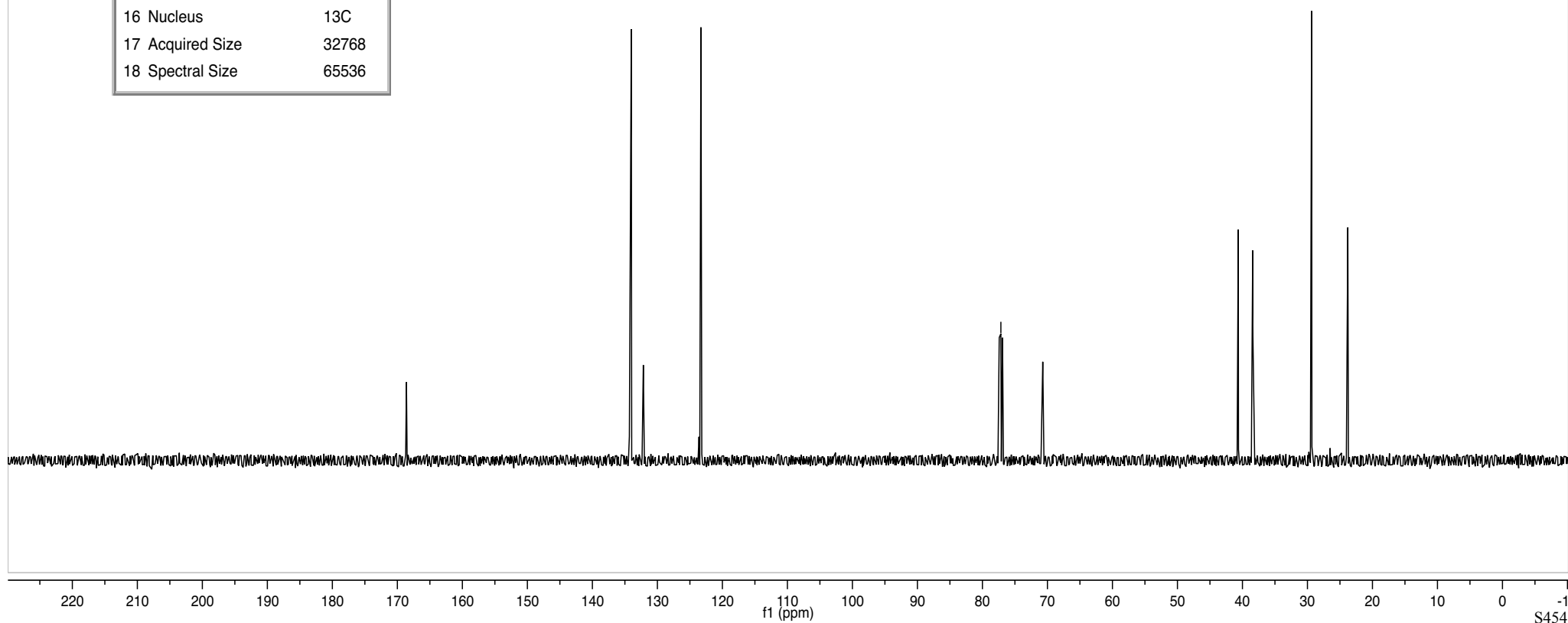
1.86
1.79
1.77
1.76
1.76
1.75
1.74
1.73
1.52
1.51
1.50
1.49
1.48
1.19

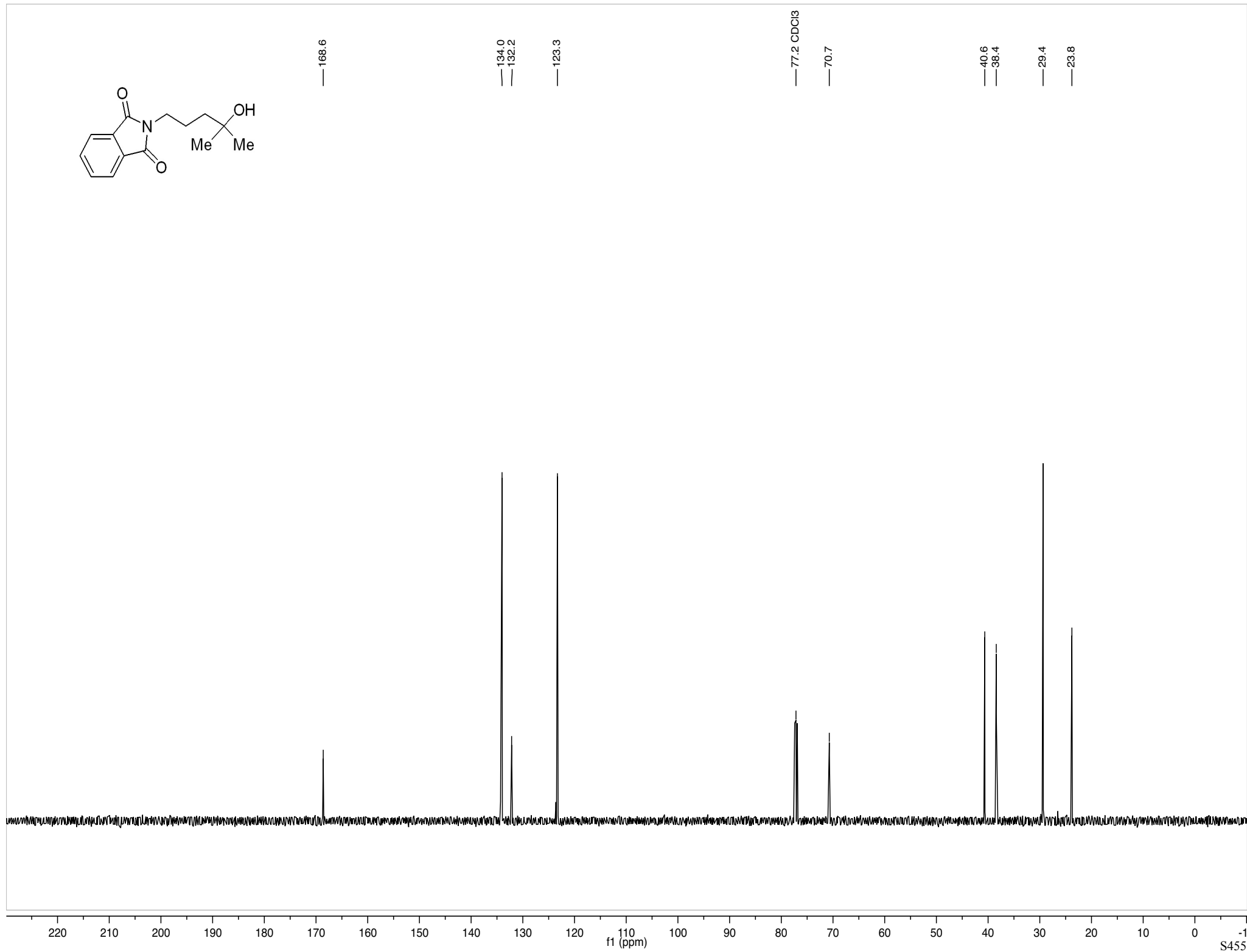
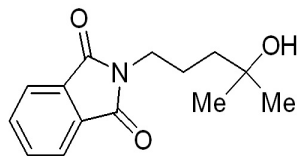




— 77.2 CDCl₃

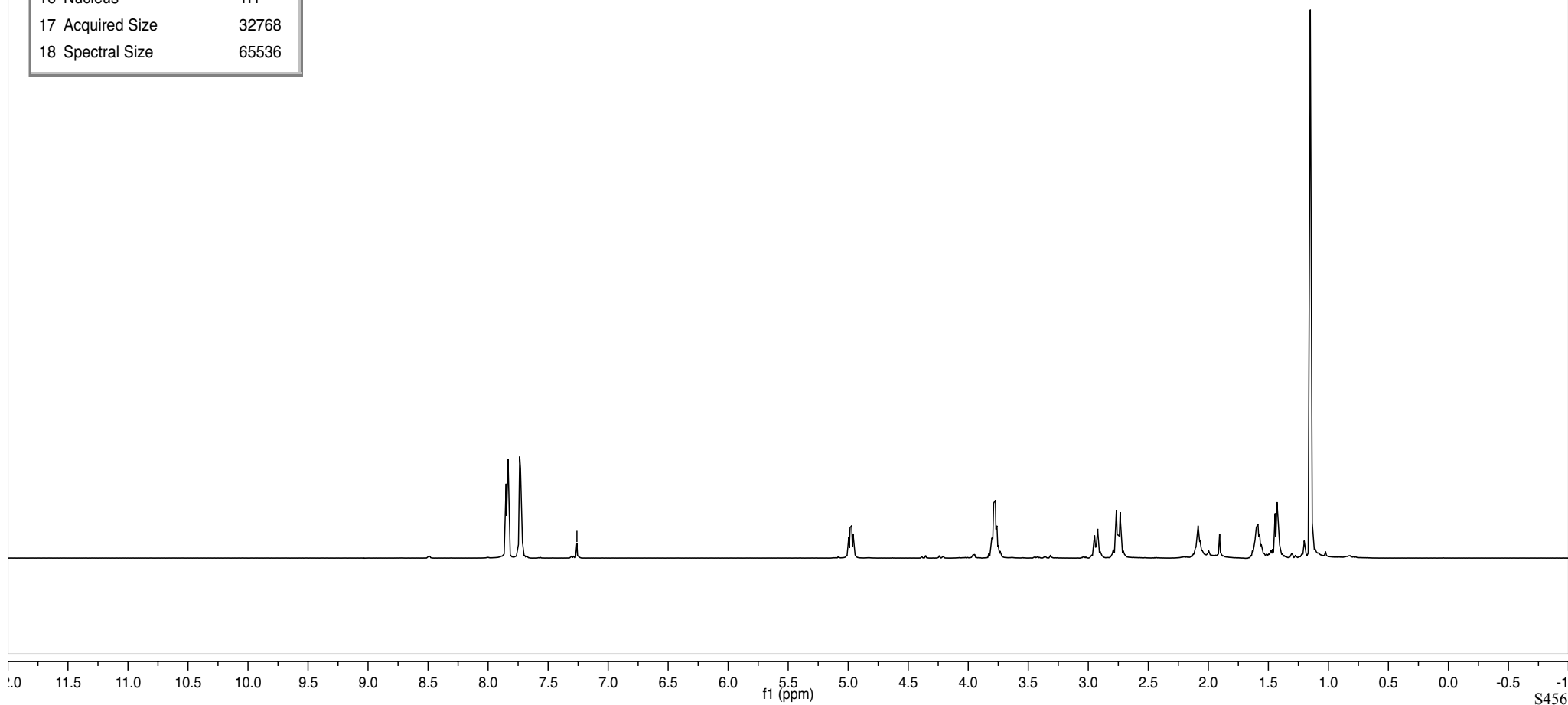
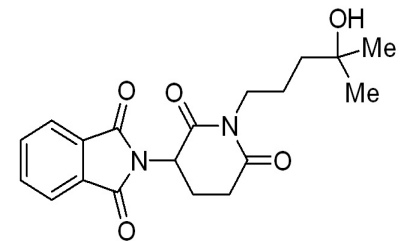
	Parameter	Value
1	Origin	Varian
2	Spectrometer	inova
3	Solvent	CDCl ₃
4	Temperature	40.0
5	Pulse Sequence	s2pul
6	Experiment	1D
7	Probe	QUAD
8	Number of Scans	64
9	Receiver Gain	60
10	Relaxation Delay	1.0000
11	Pulse Width	0.0000
12	Acquisition Time	1.0863
13	Spectrometer Frequency	125.66
14	Spectral Width	30165.9
15	Lowest Frequency	-1260.2
16	Nucleus	¹³ C
17	Acquired Size	32768
18	Spectral Size	65536

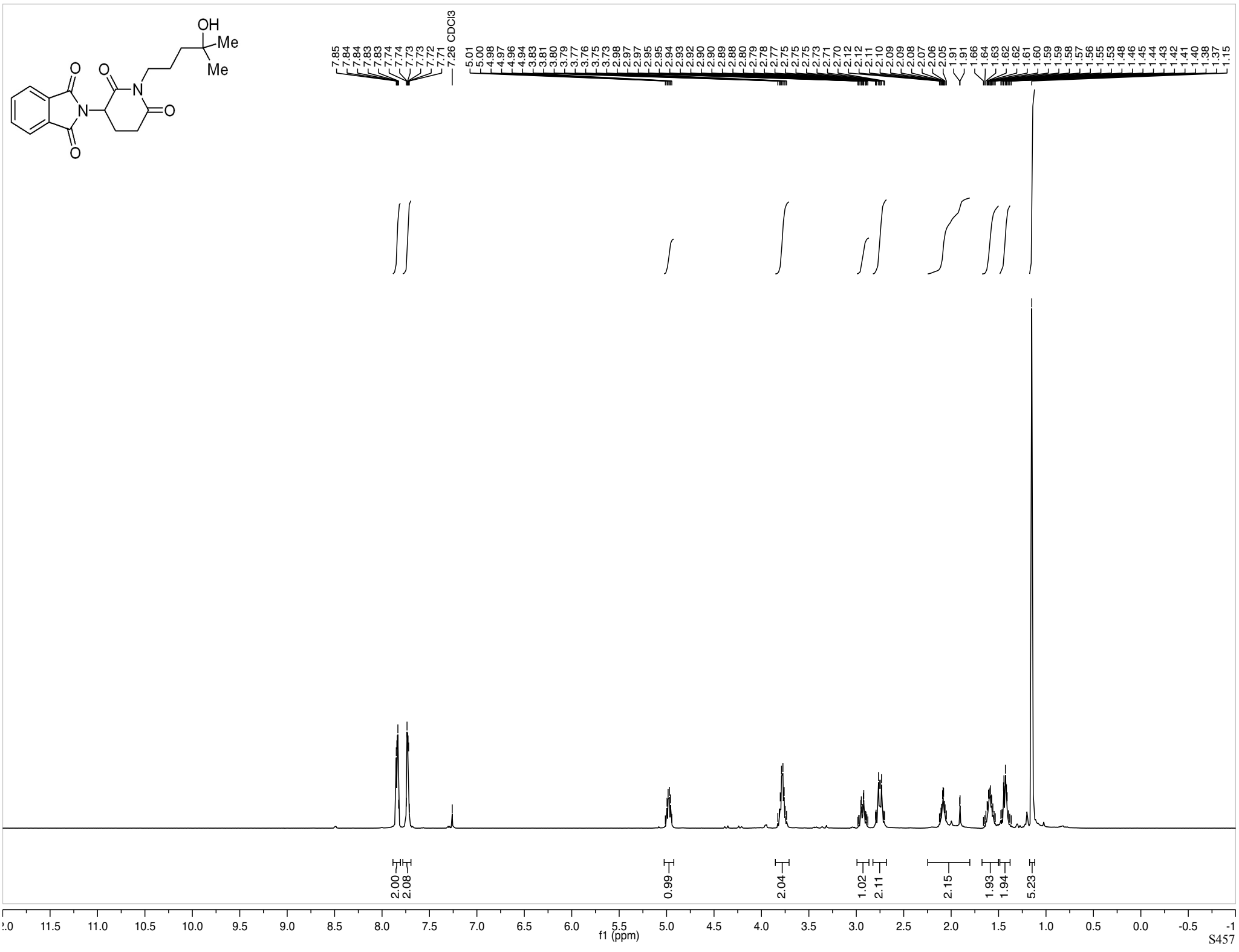




Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	8
9 Receiver Gain	41
10 Relaxation Delay	0.0000
11 Pulse Width	0.0000
12 Acquisition Time	4.6645
13 Spectrometer Frequency	499.69
14 Spectral Width	7024.9
15 Lowest Frequency	-1021.4
16 Nucleus	¹ H
17 Acquired Size	32768
18 Spectral Size	65536

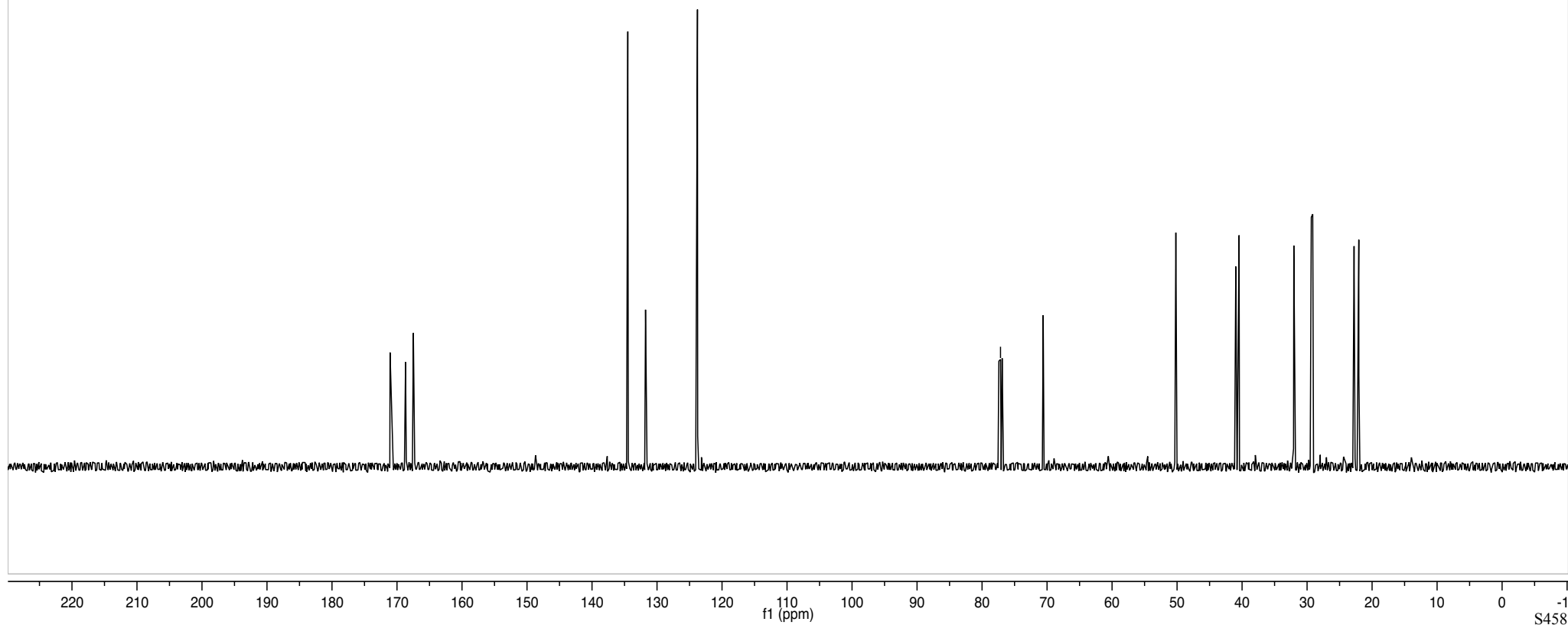
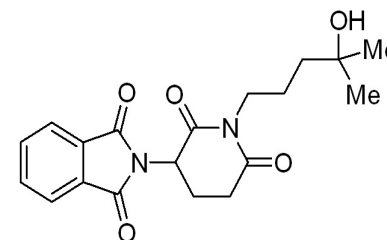
—7.3 CDCl3

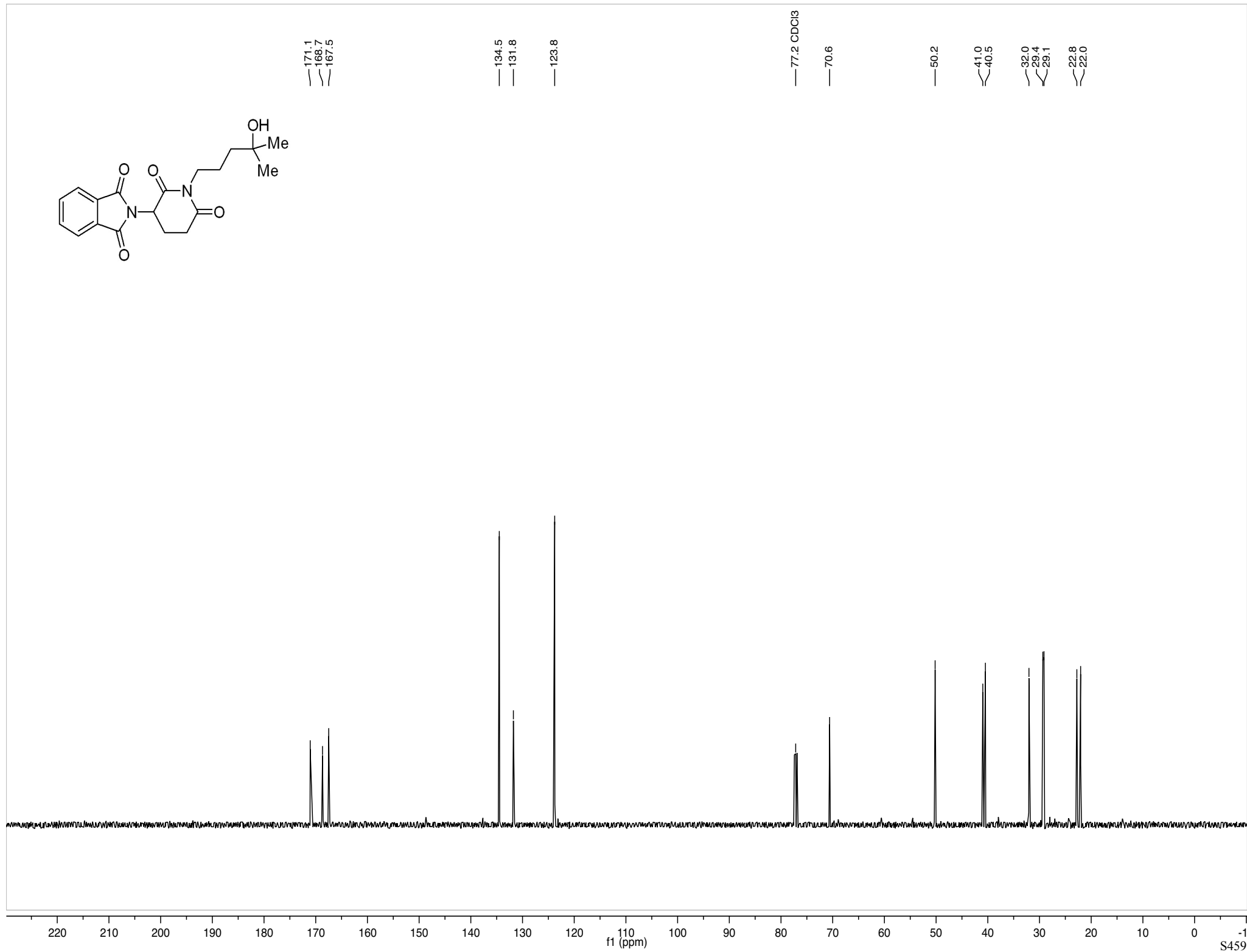
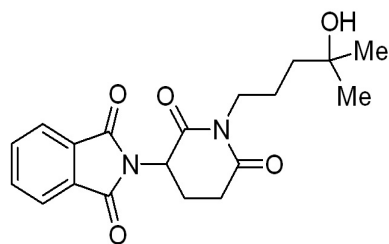




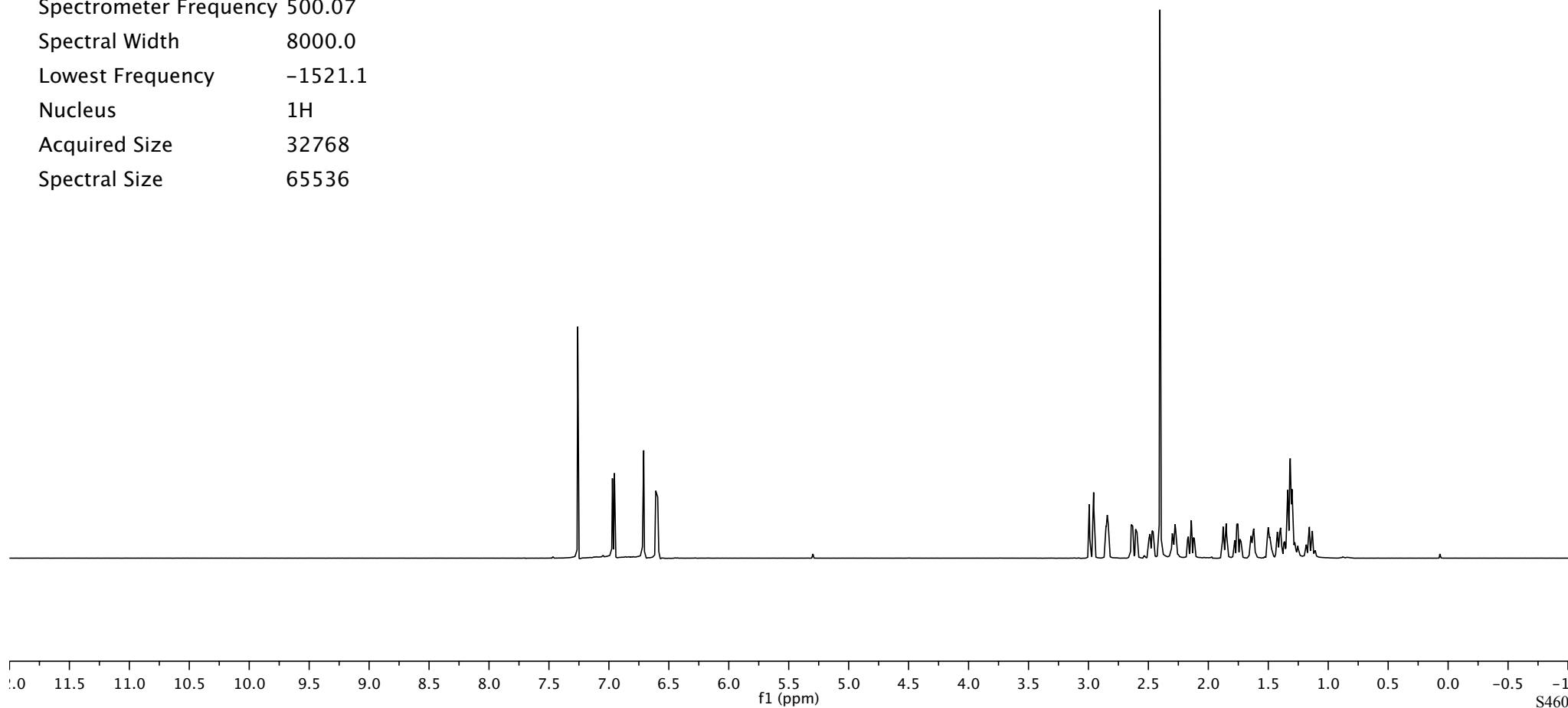
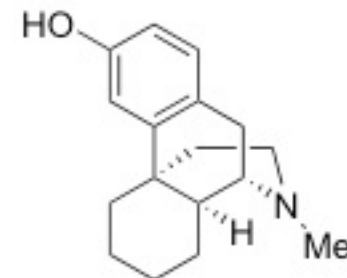
Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	112
9 Receiver Gain	60
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.0863
13 Spectrometer Frequency	125.66
14 Spectral Width	30165.9
15 Lowest Frequency	-1282.7
16 Nucleus	¹³ C
17 Acquired Size	32768
18 Spectral Size	65536

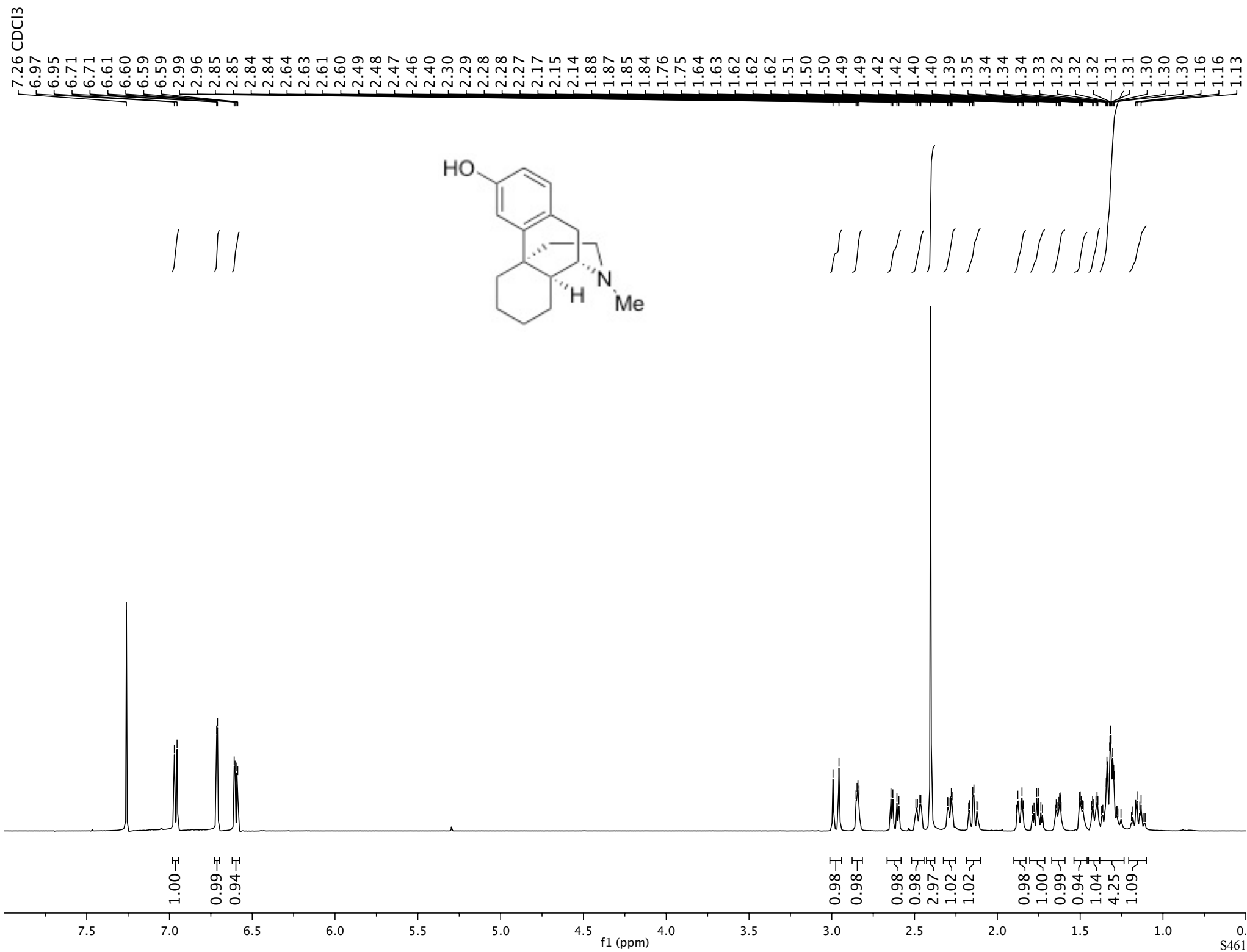
— 77.2 CDCl₃



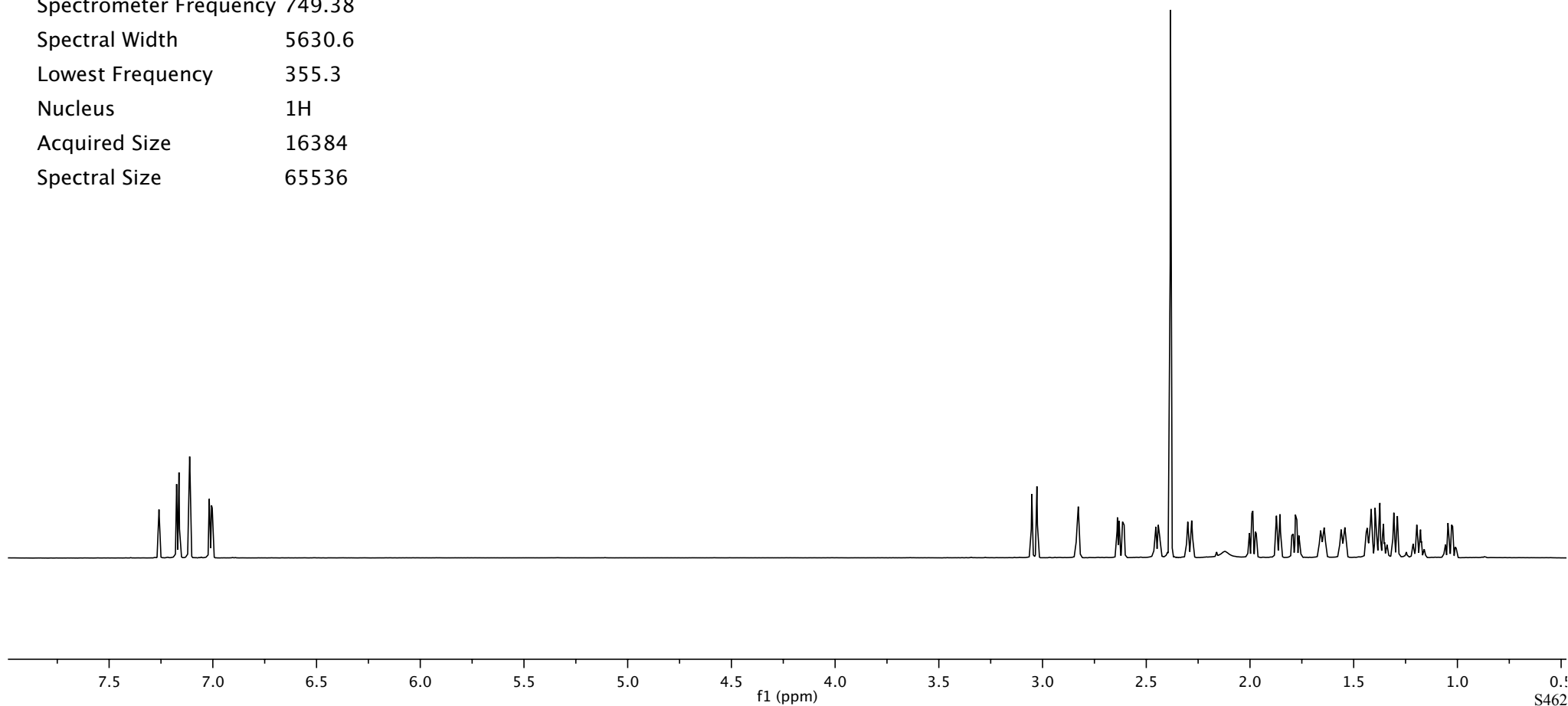
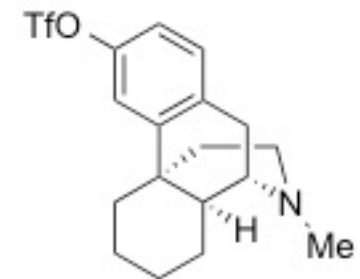


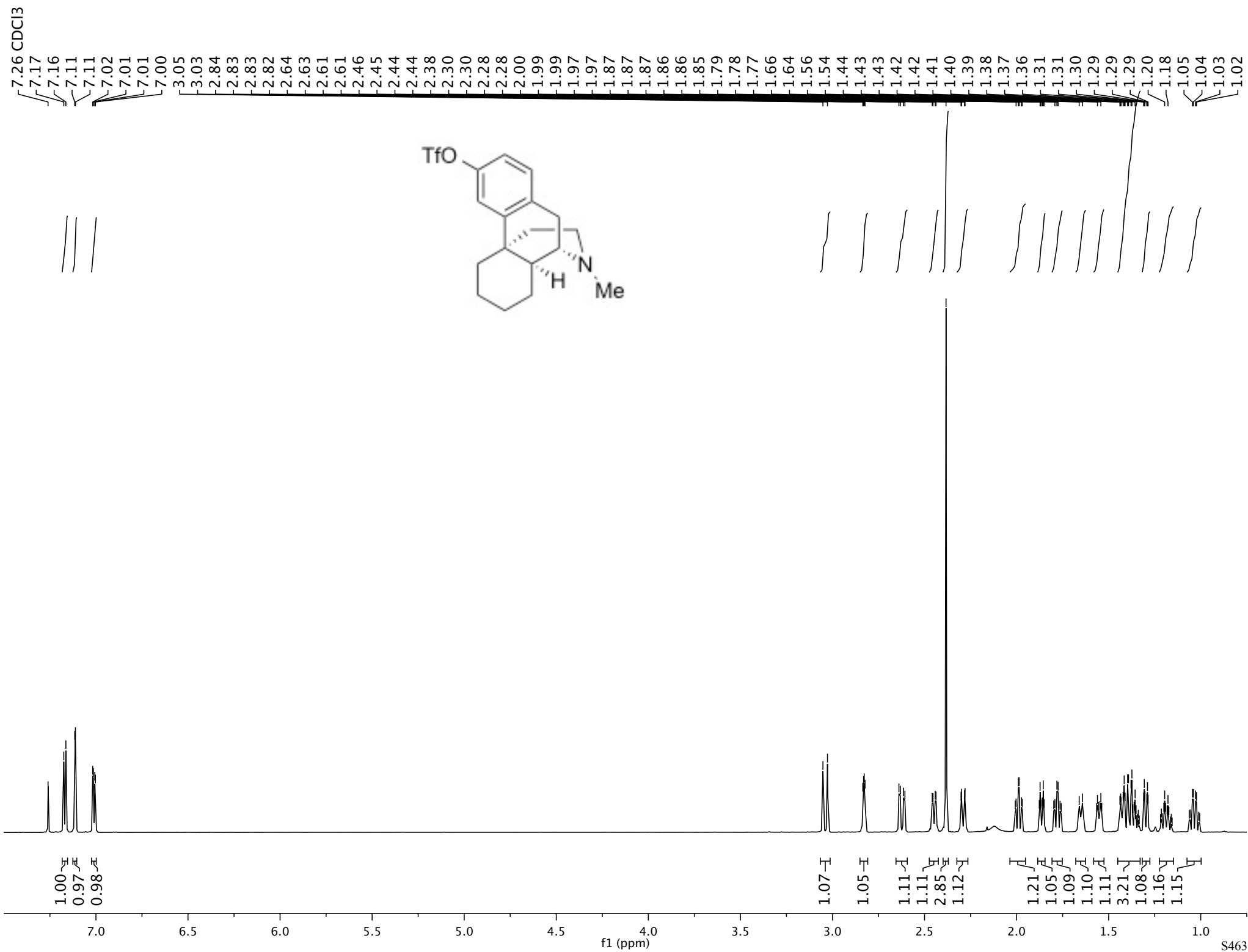
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	38
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



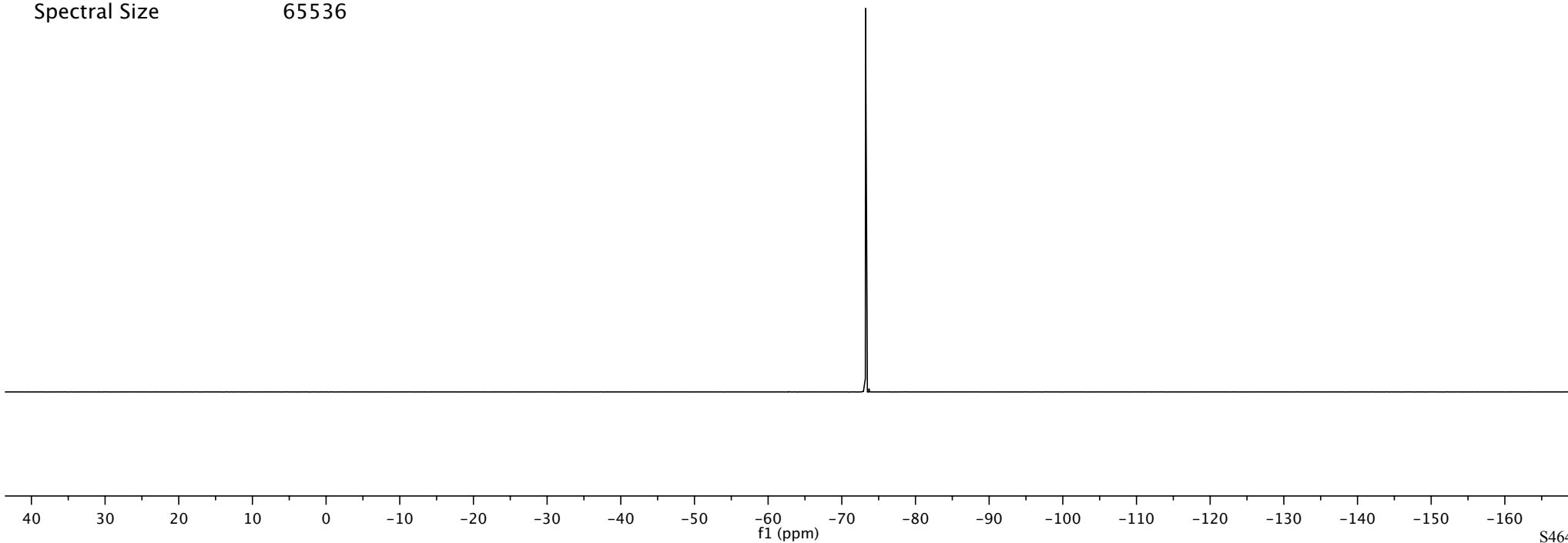
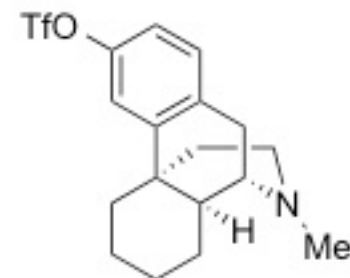


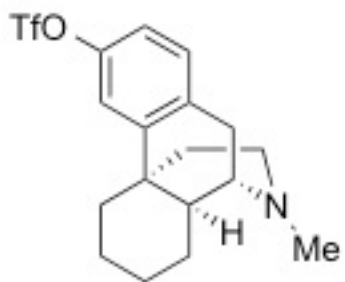
Parameter	Value
Origin	Varian
Spectrometer	vnmrs
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	triax
Number of Scans	16
Receiver Gain	18
Relaxation Delay	15.0000
Pulse Width	0.0000
Acquisition Time	2.9098
Spectrometer Frequency	749.38
Spectral Width	5630.6
Lowest Frequency	355.3
Nucleus	¹ H
Acquired Size	16384
Spectral Size	65536



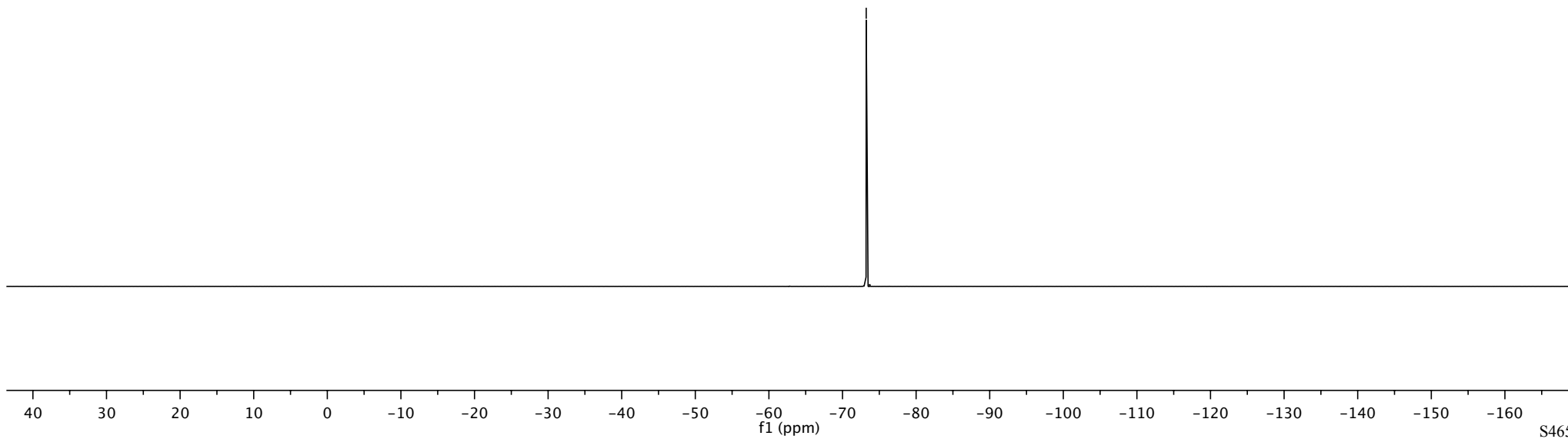


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	128
Receiver Gain	52
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency	-79501.3
Nucleus	¹⁹ F
Acquired Size	32768
Spectral Size	65536

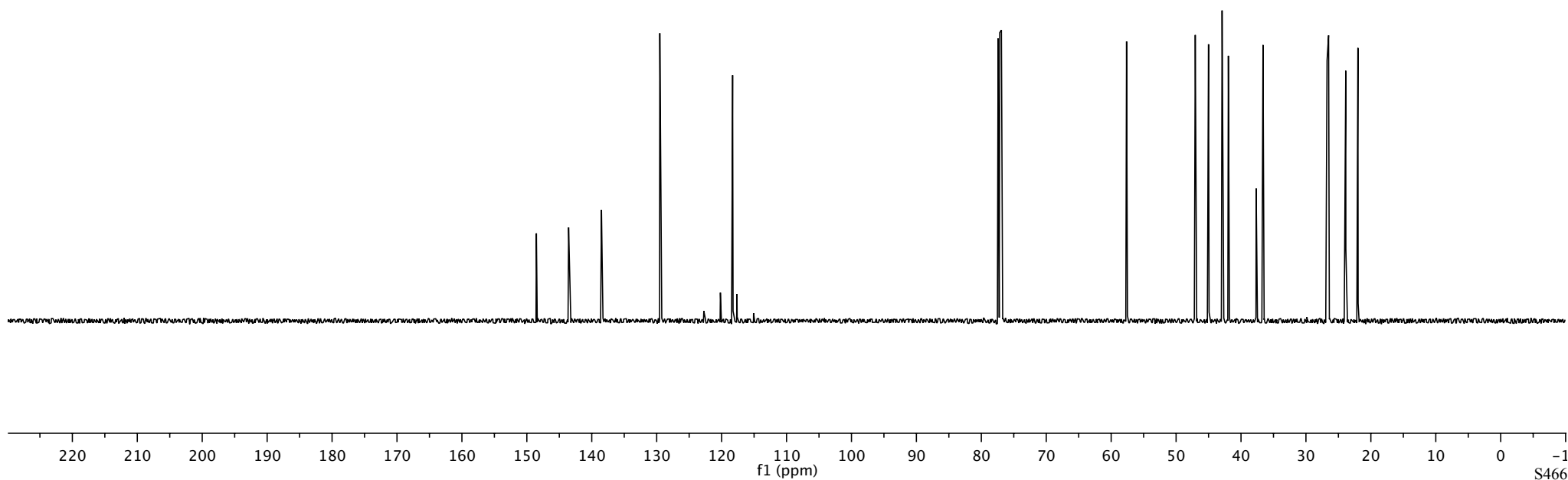
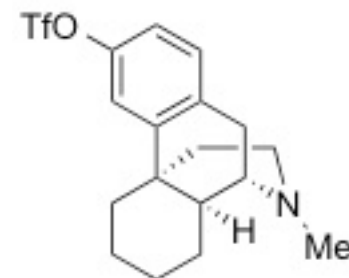


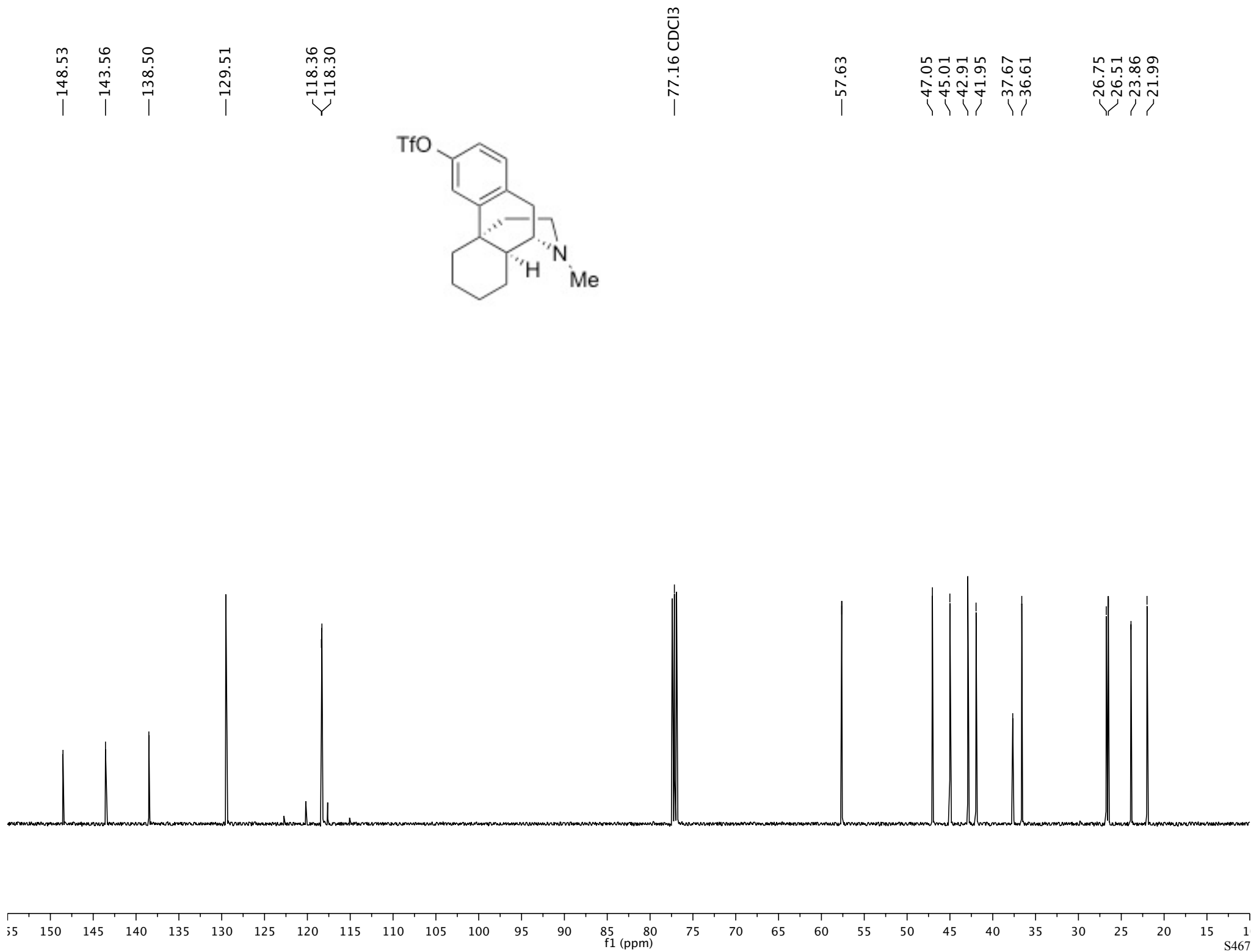


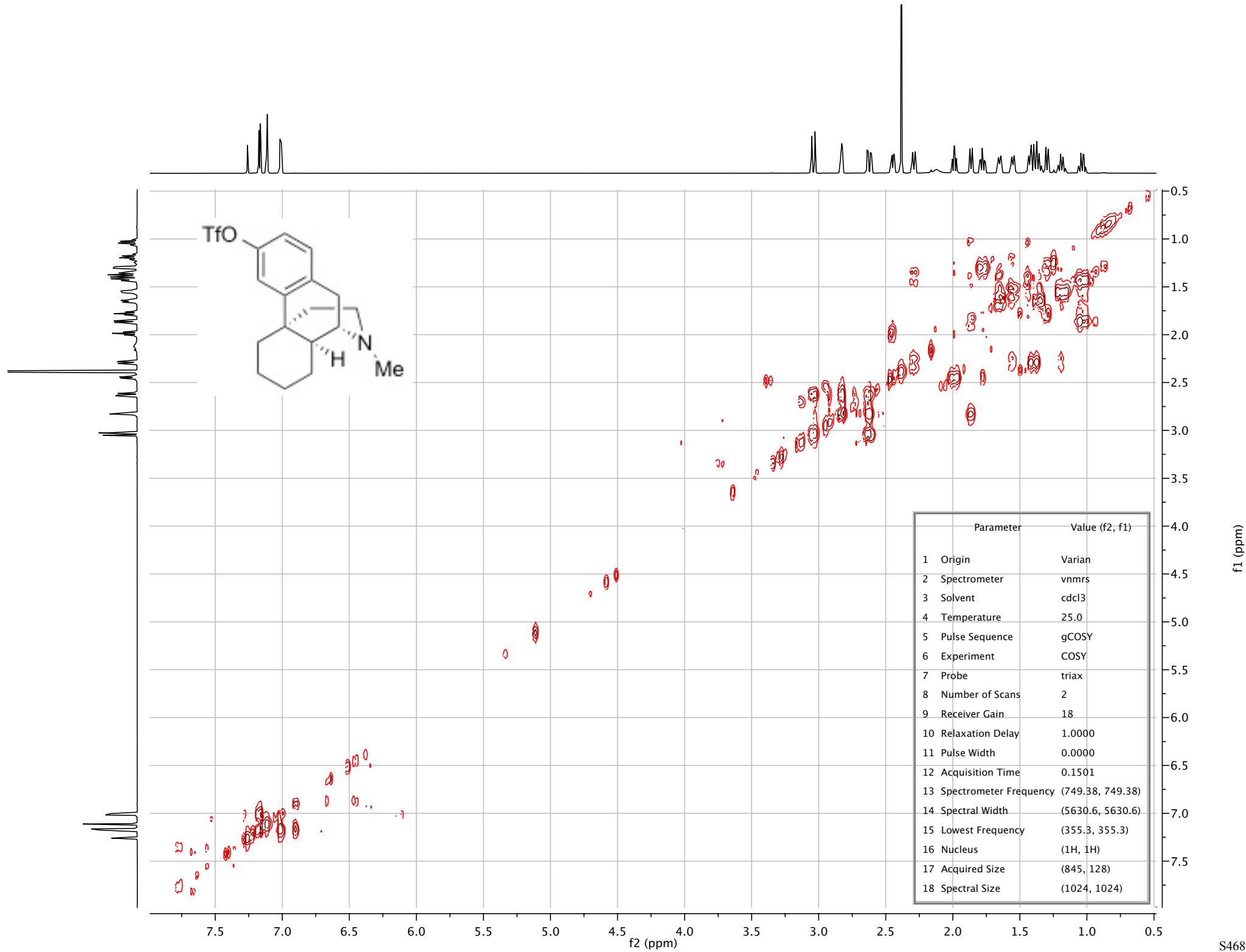
--73.22

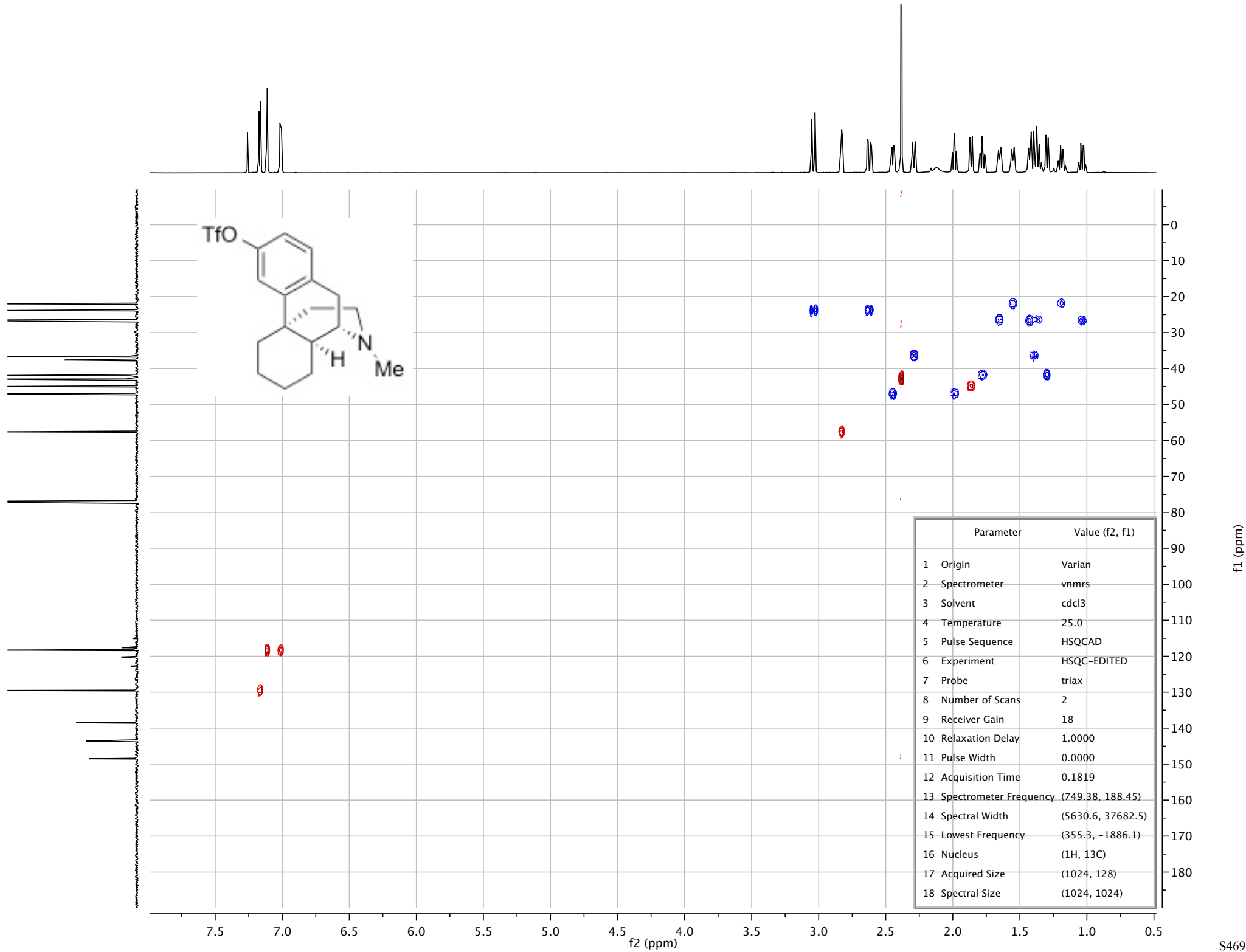


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	1326
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1273.0
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

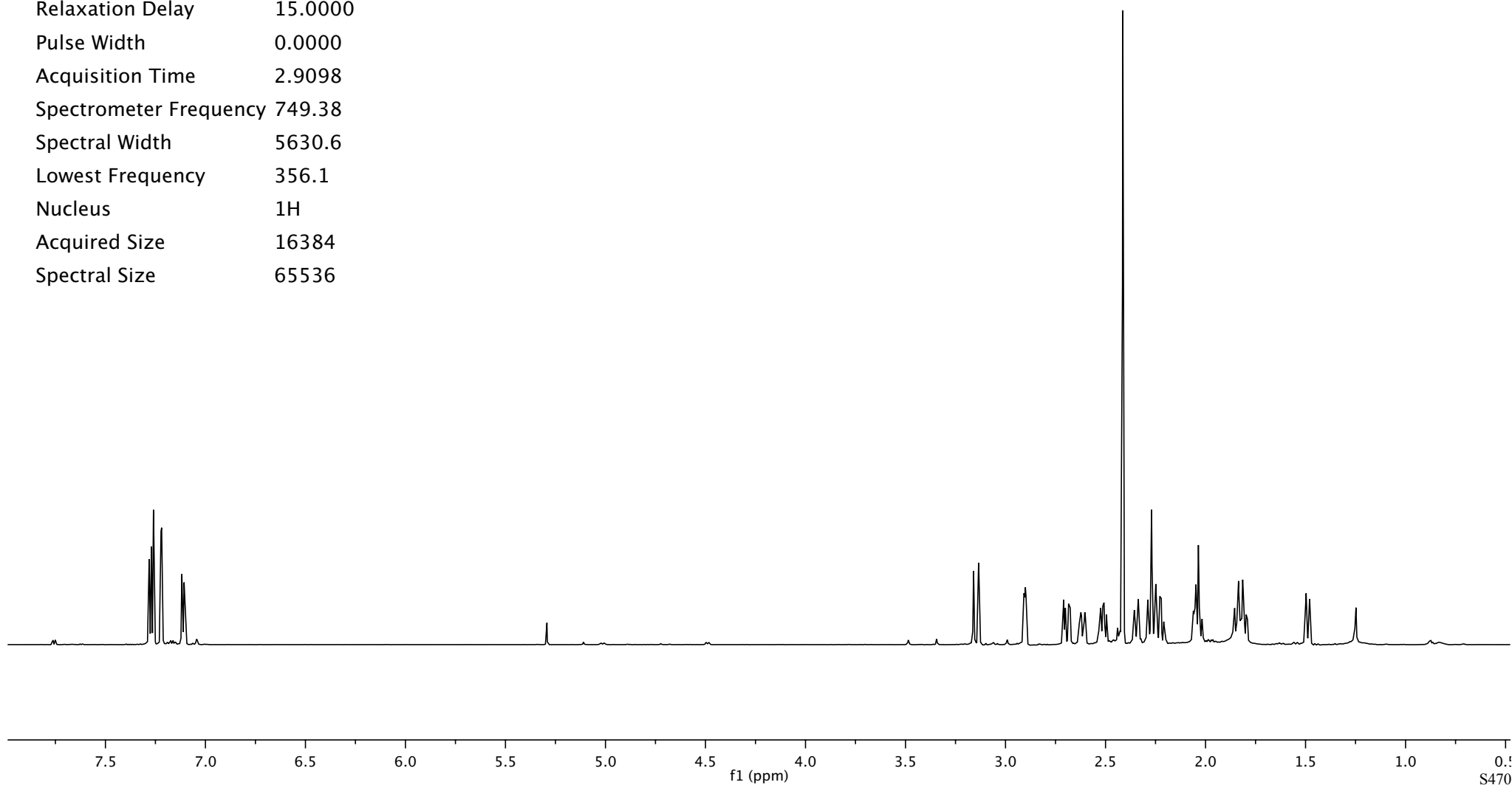
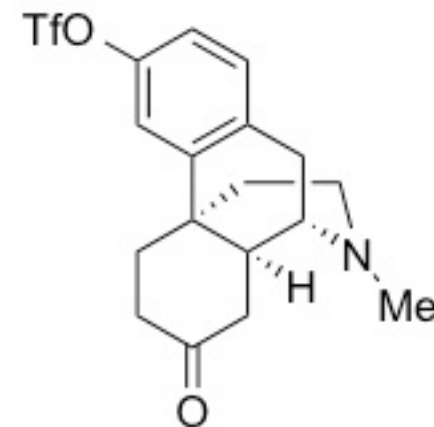


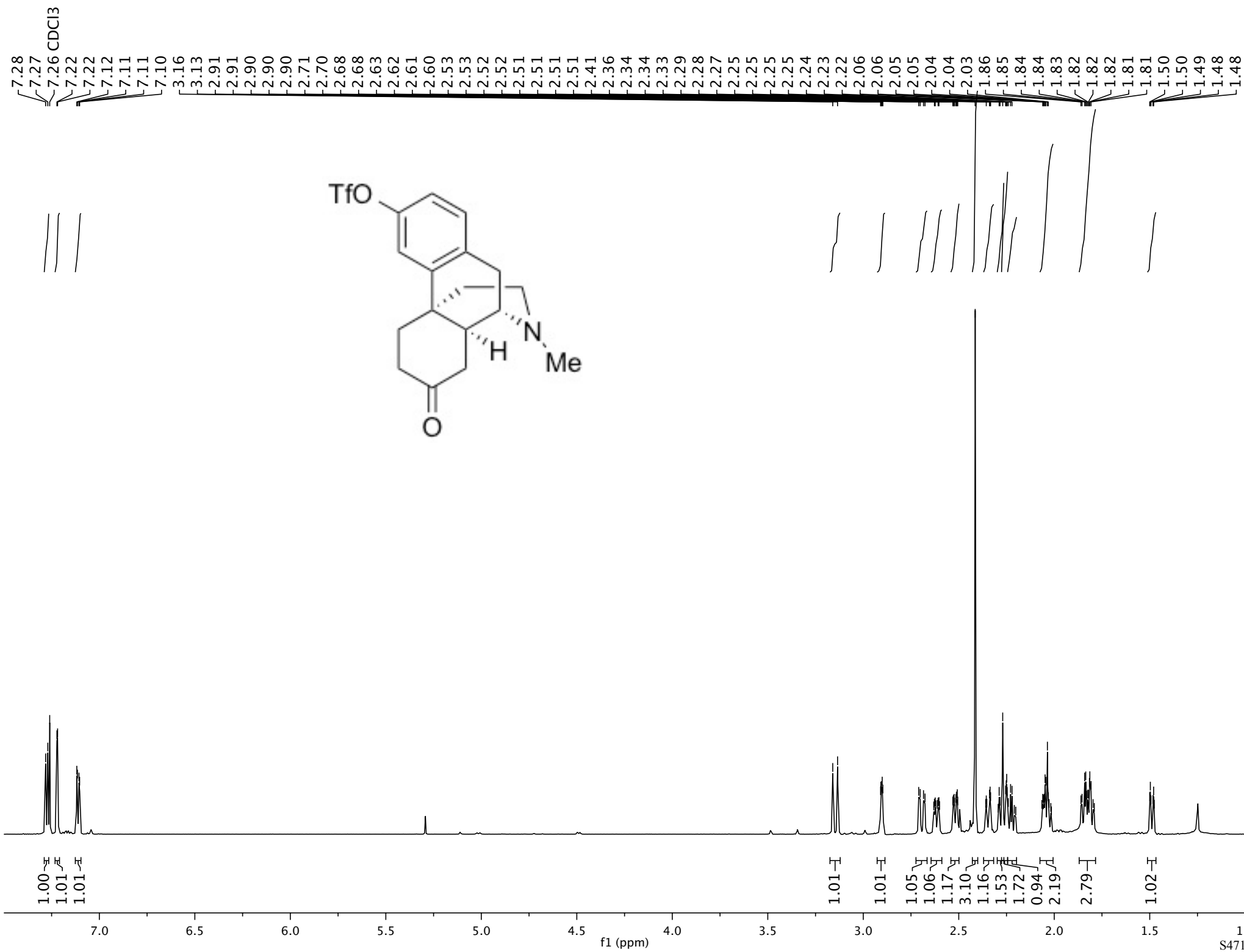




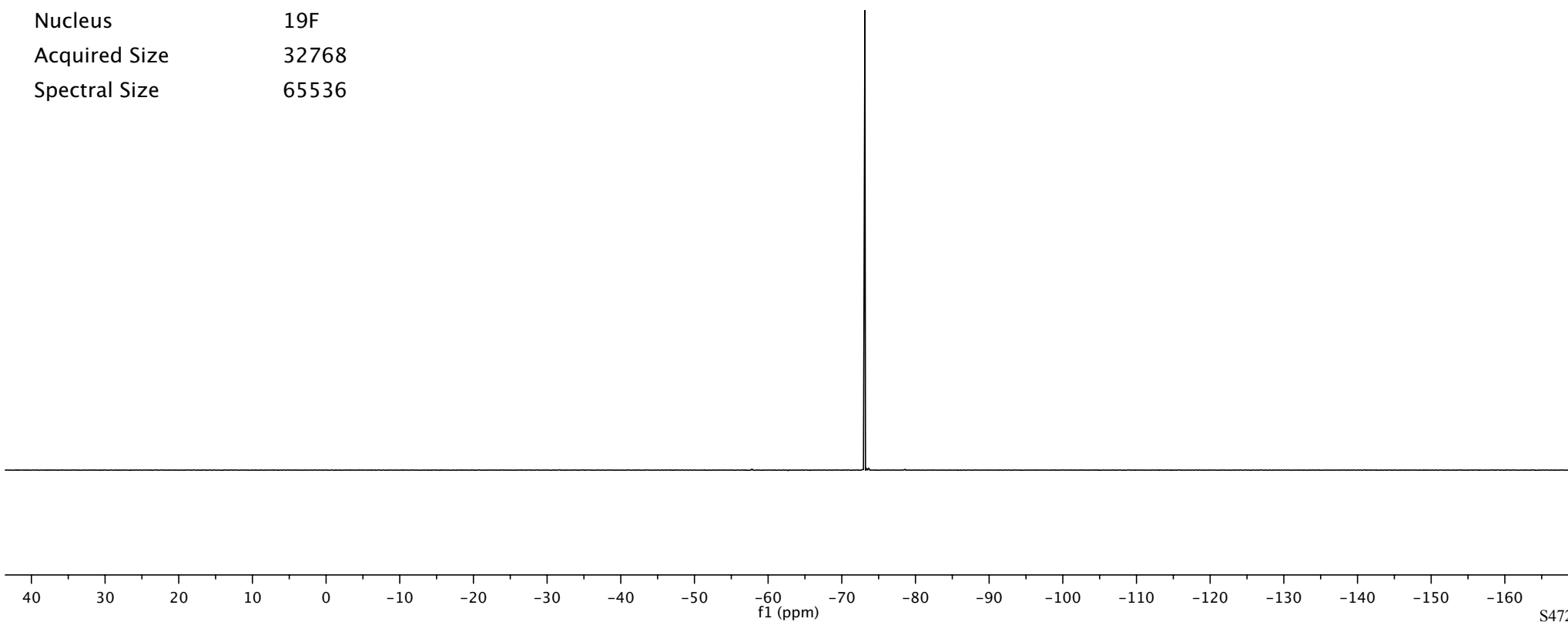
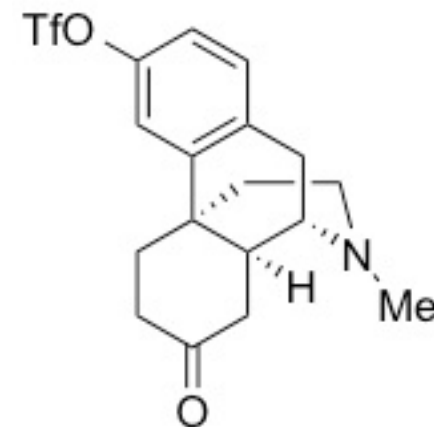


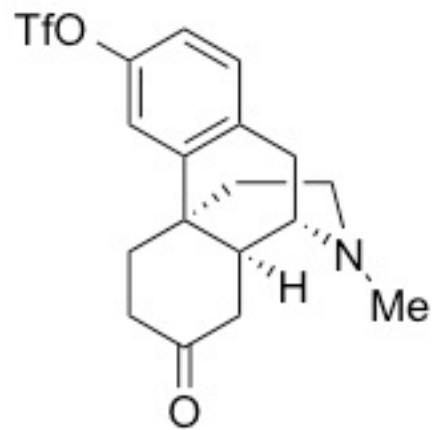
Parameter	Value
Origin	Varian
Spectrometer	vnmrs
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	triax
Number of Scans	16
Receiver Gain	32
Relaxation Delay	15.0000
Pulse Width	0.0000
Acquisition Time	2.9098
Spectrometer Frequency	749.38
Spectral Width	5630.6
Lowest Frequency	356.1
Nucleus	¹ H
Acquired Size	16384
Spectral Size	65536



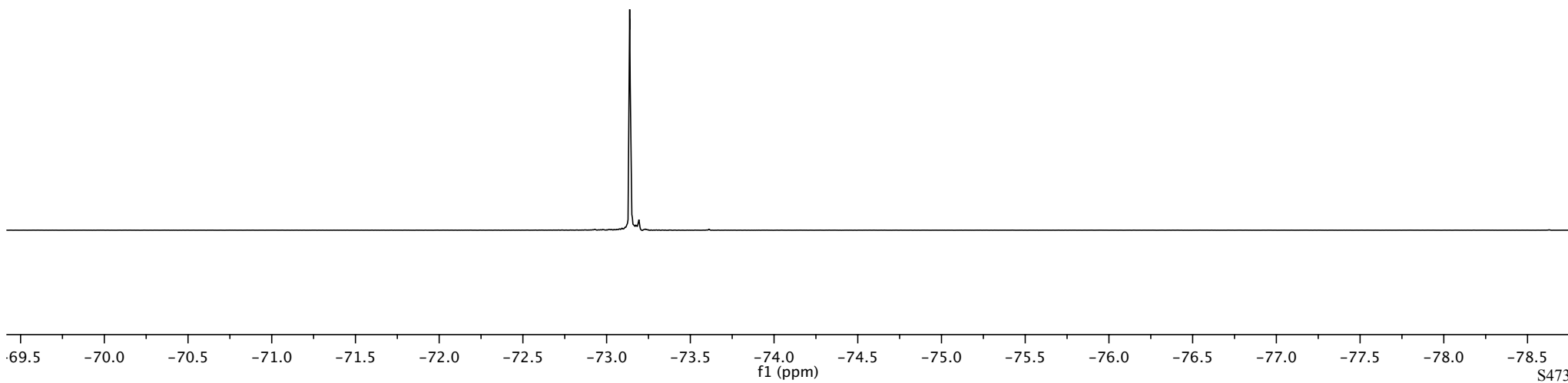


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	128
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency	-79501.3
Nucleus	19F
Acquired Size	32768
Spectral Size	65536



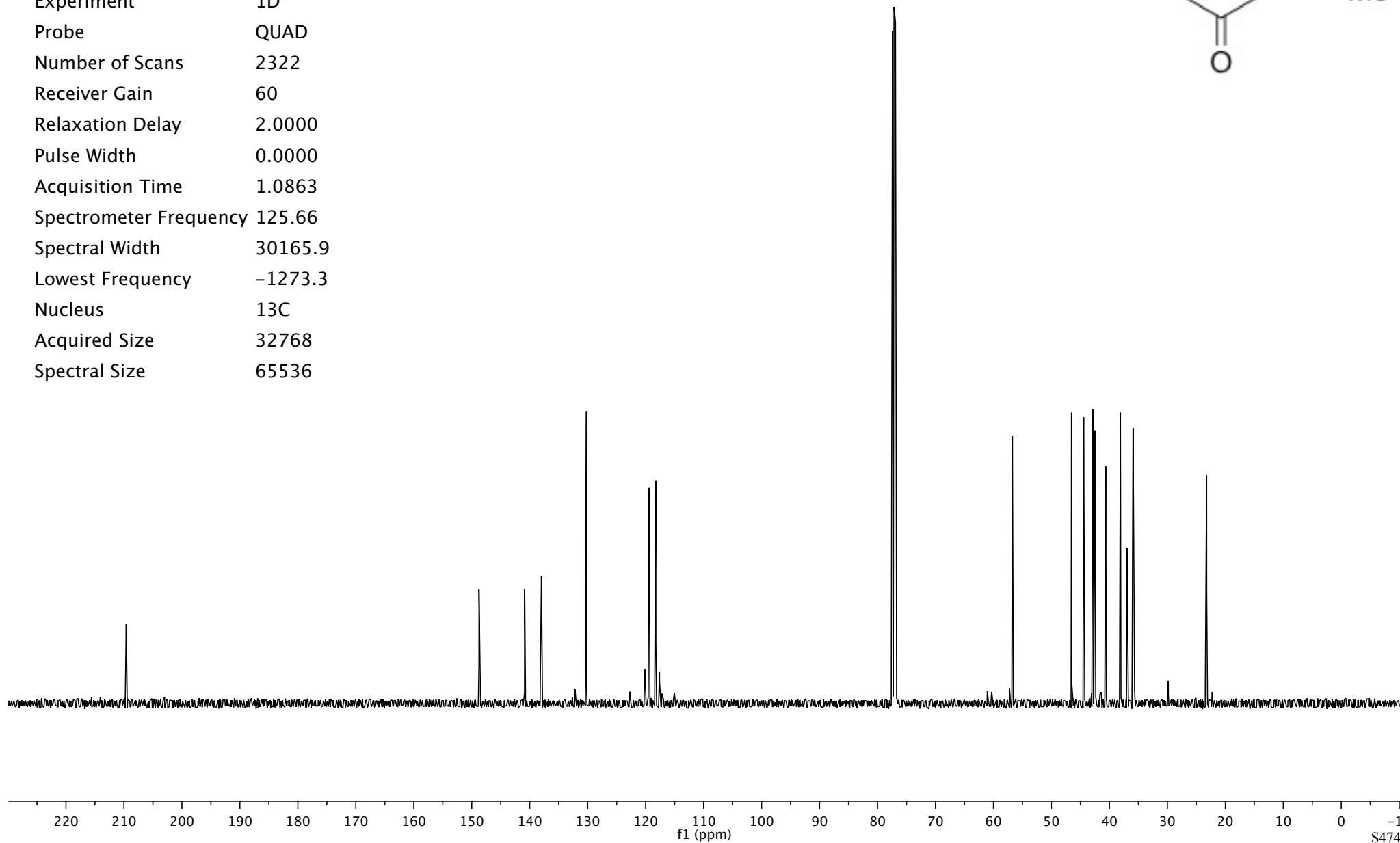
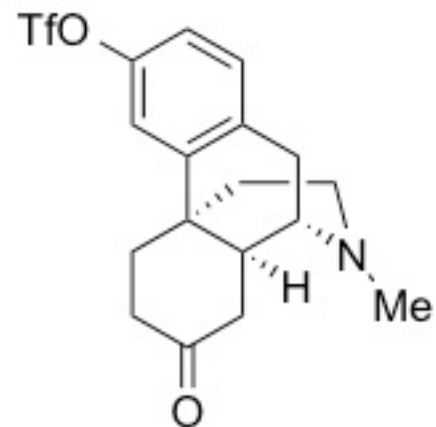


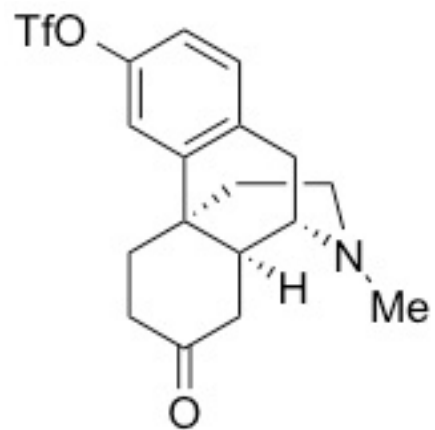
--73.14



JMH-V-141C.1_13C
8.14.2015
JMH-V-141C.1

Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	2322
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1273.3
Nucleus	13C
Acquired Size	32768
Spectral Size	65536





—209.61

—148.75

—140.87

—137.98

—130.22

—122.71

—120.16

—119.42

—118.25

—117.61

—115.05

—77.16 CDCl₃

—56.73

—46.53

—44.44

—42.81

—42.52

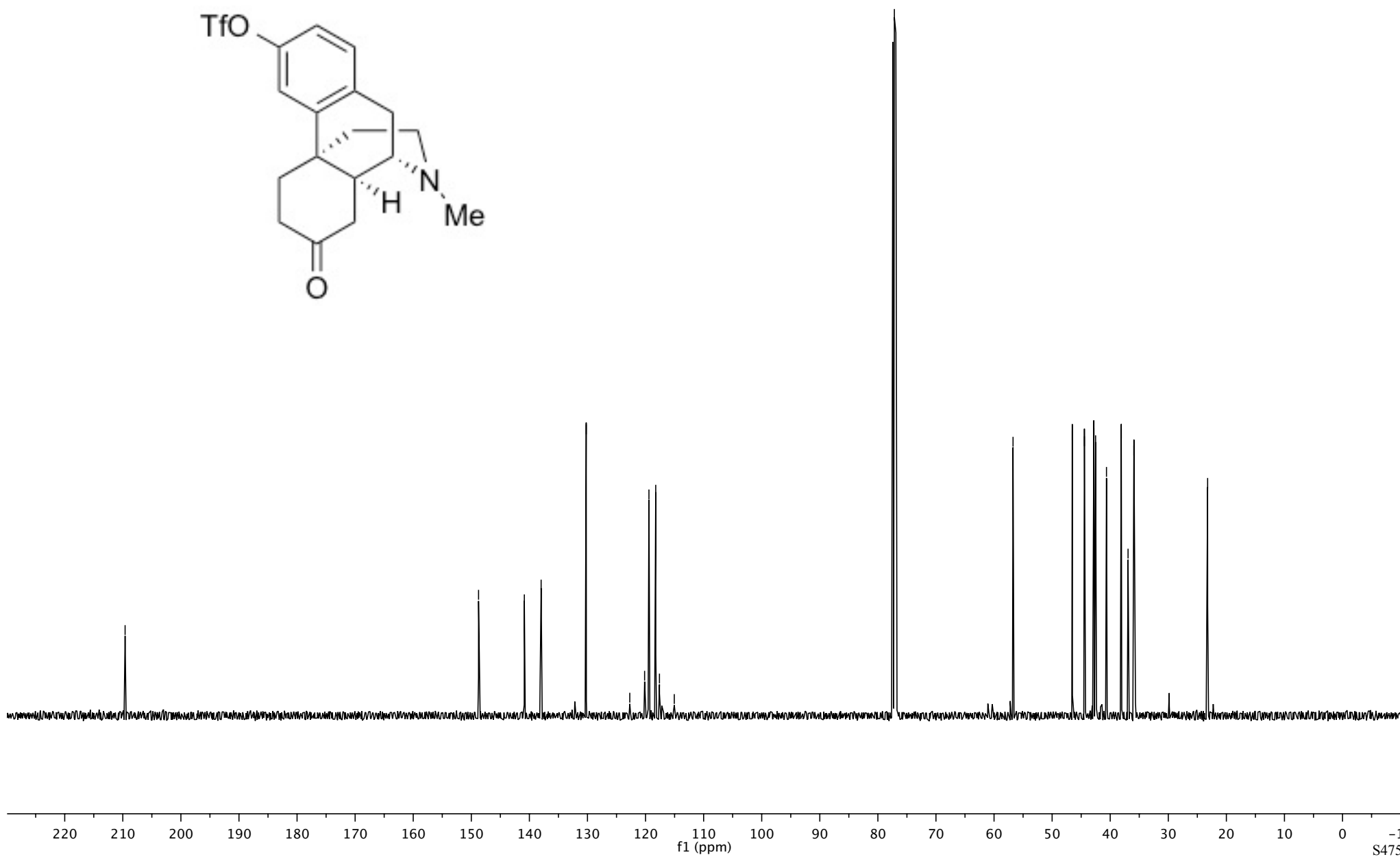
—40.64

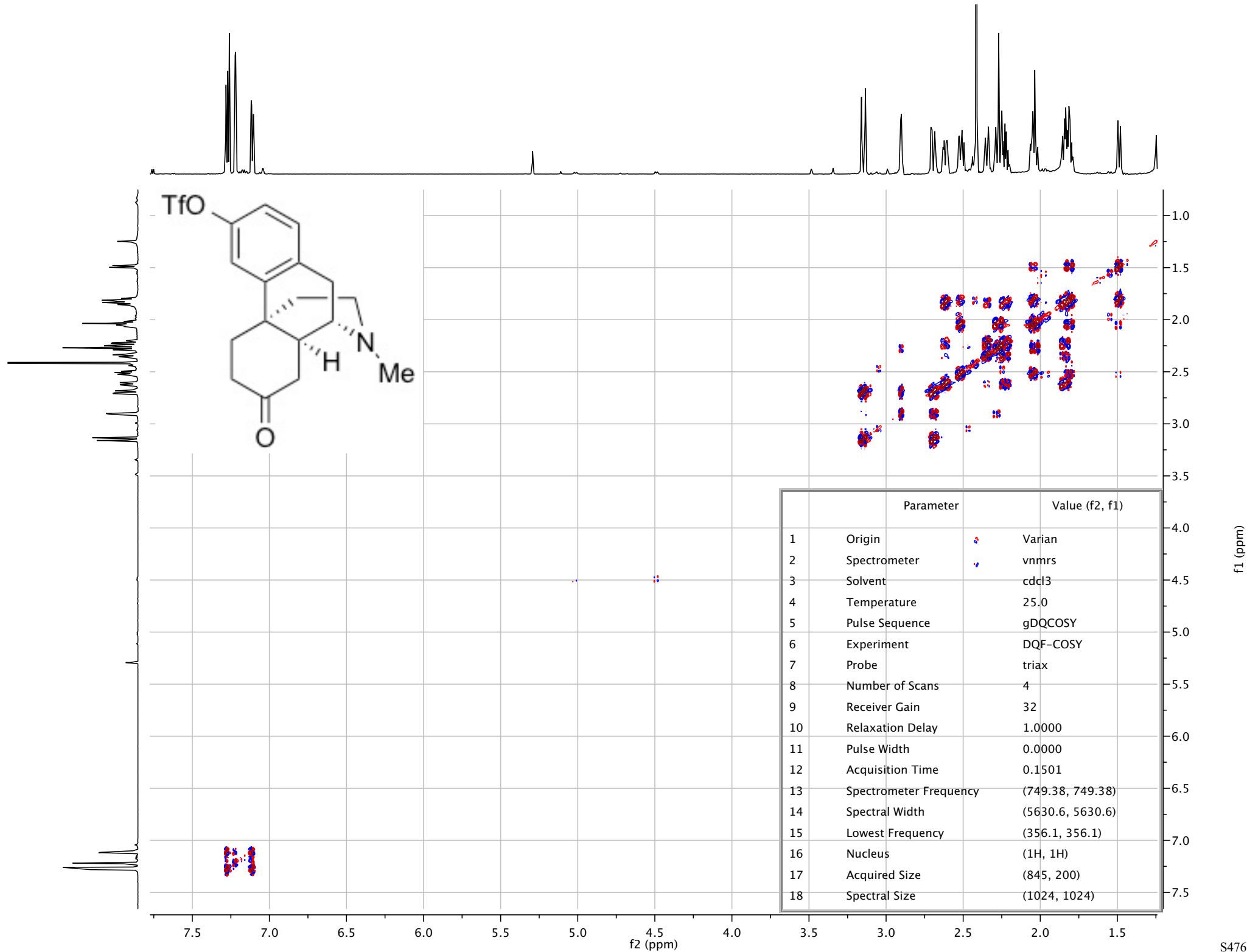
—38.10

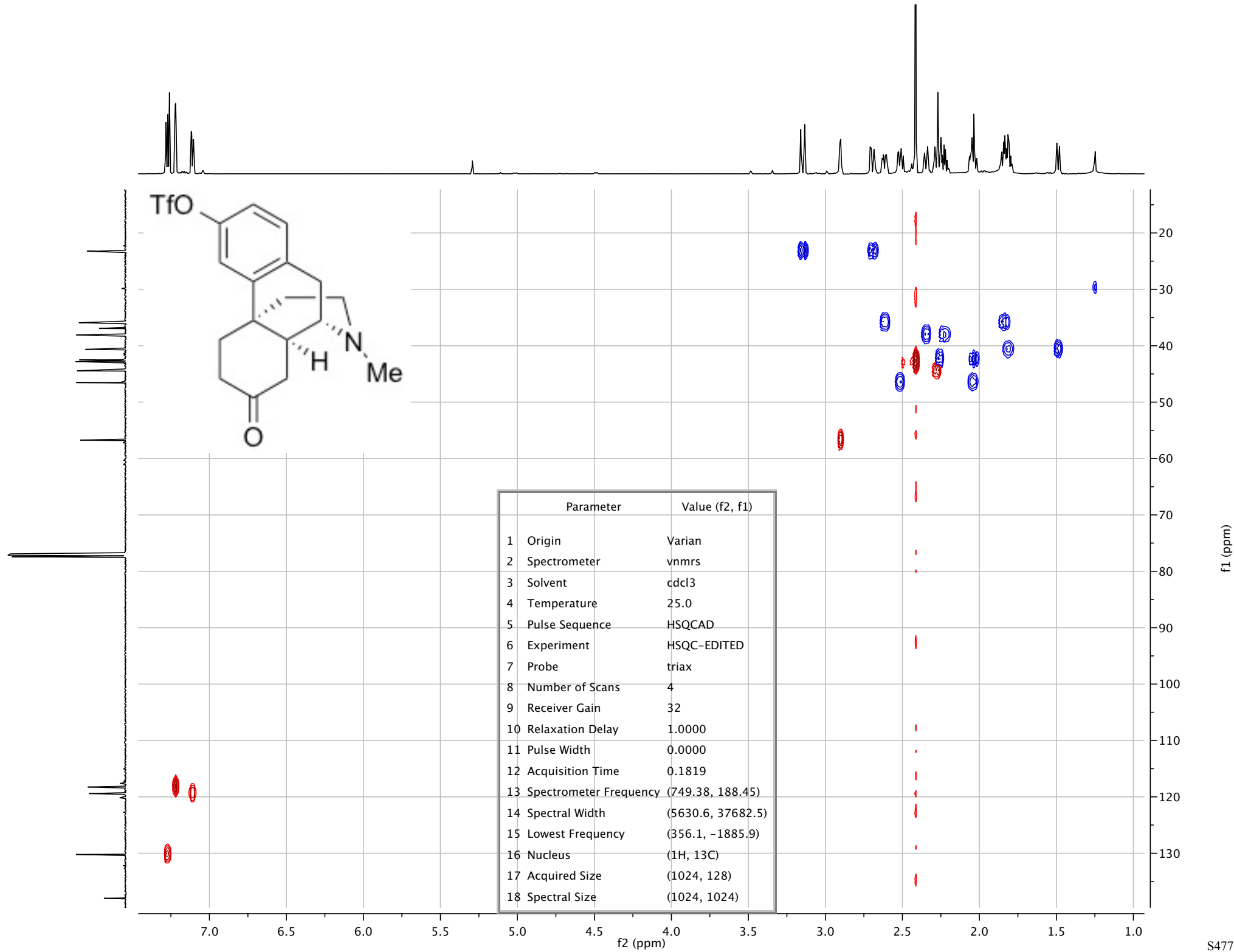
—36.93

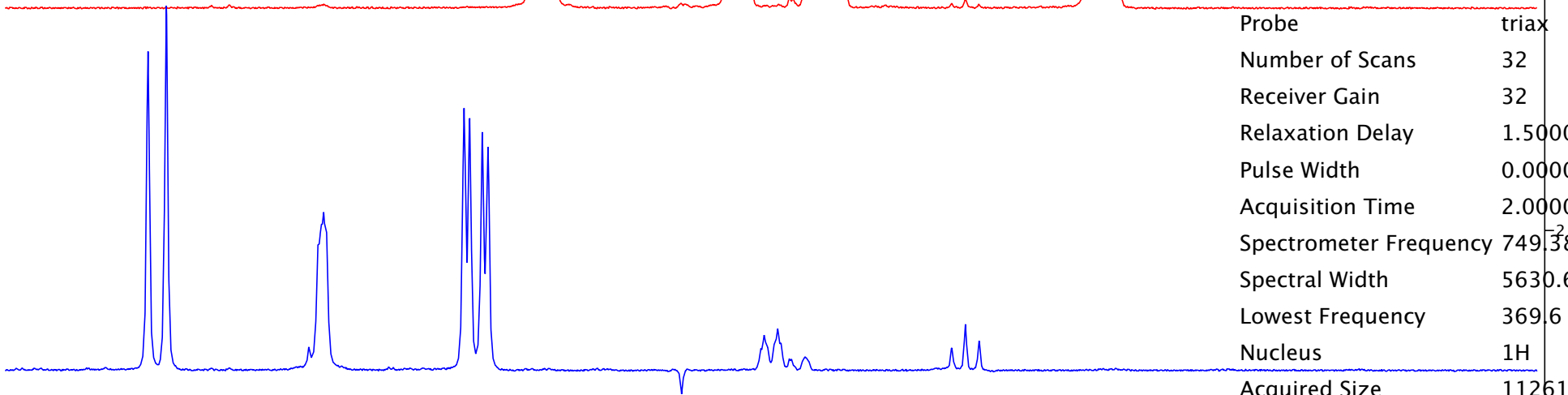
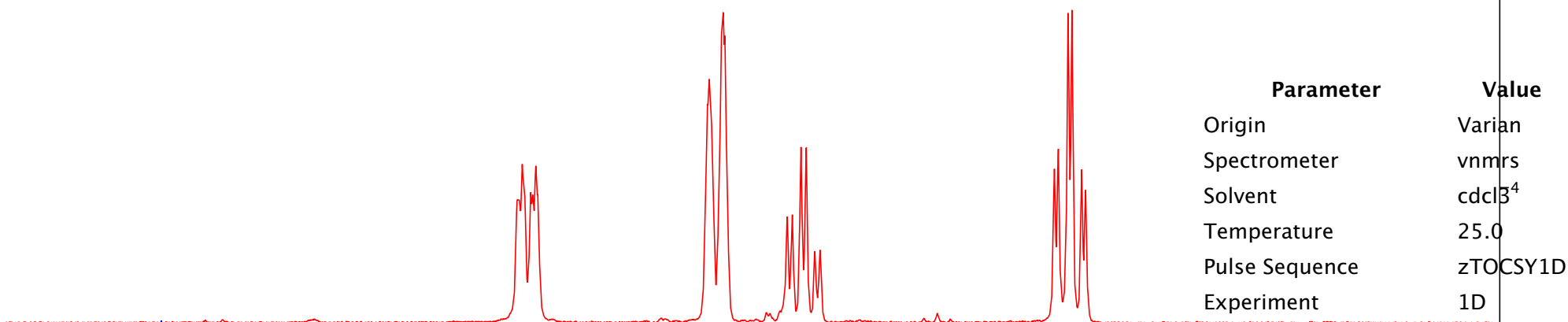
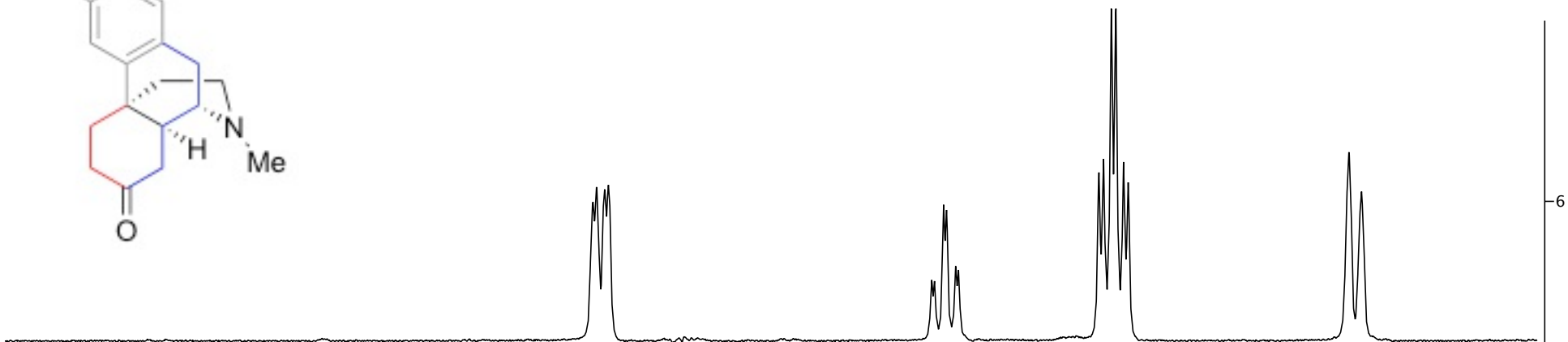
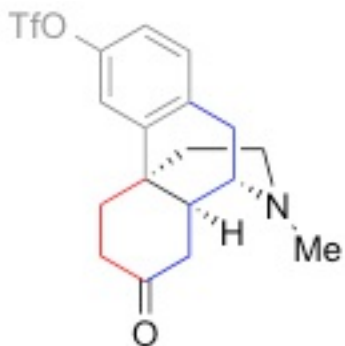
—35.92

—23.23



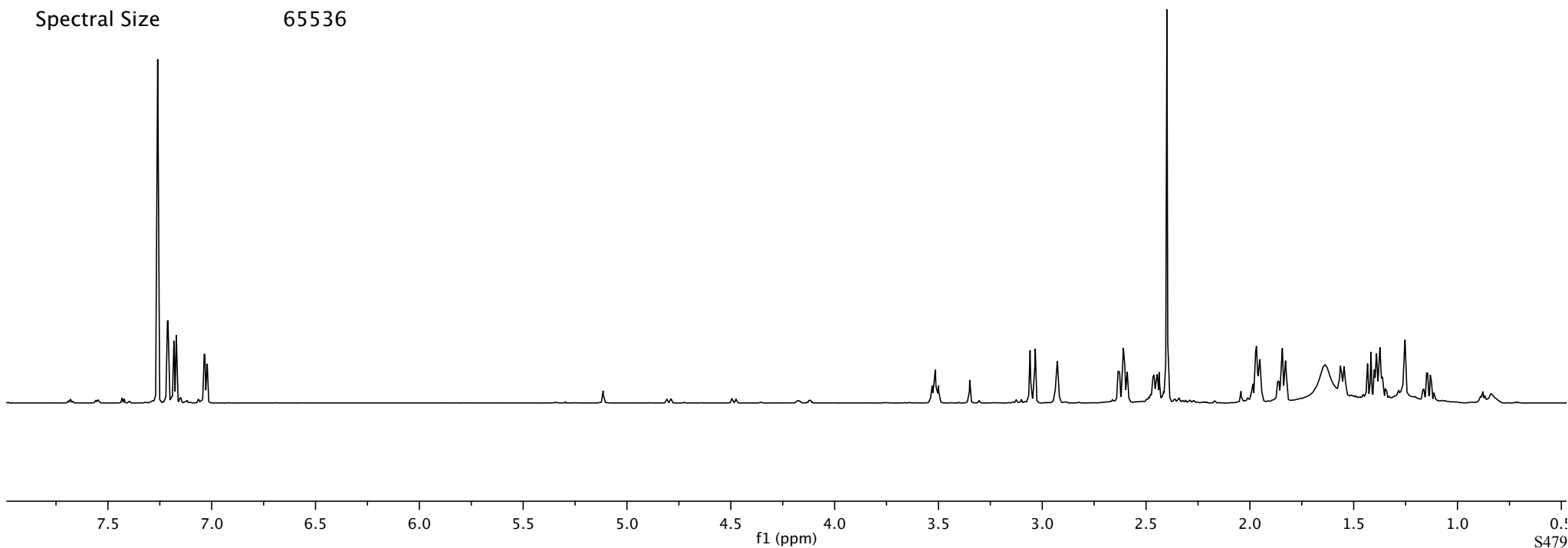
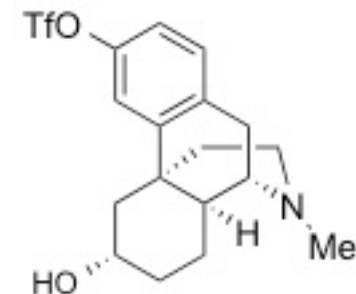


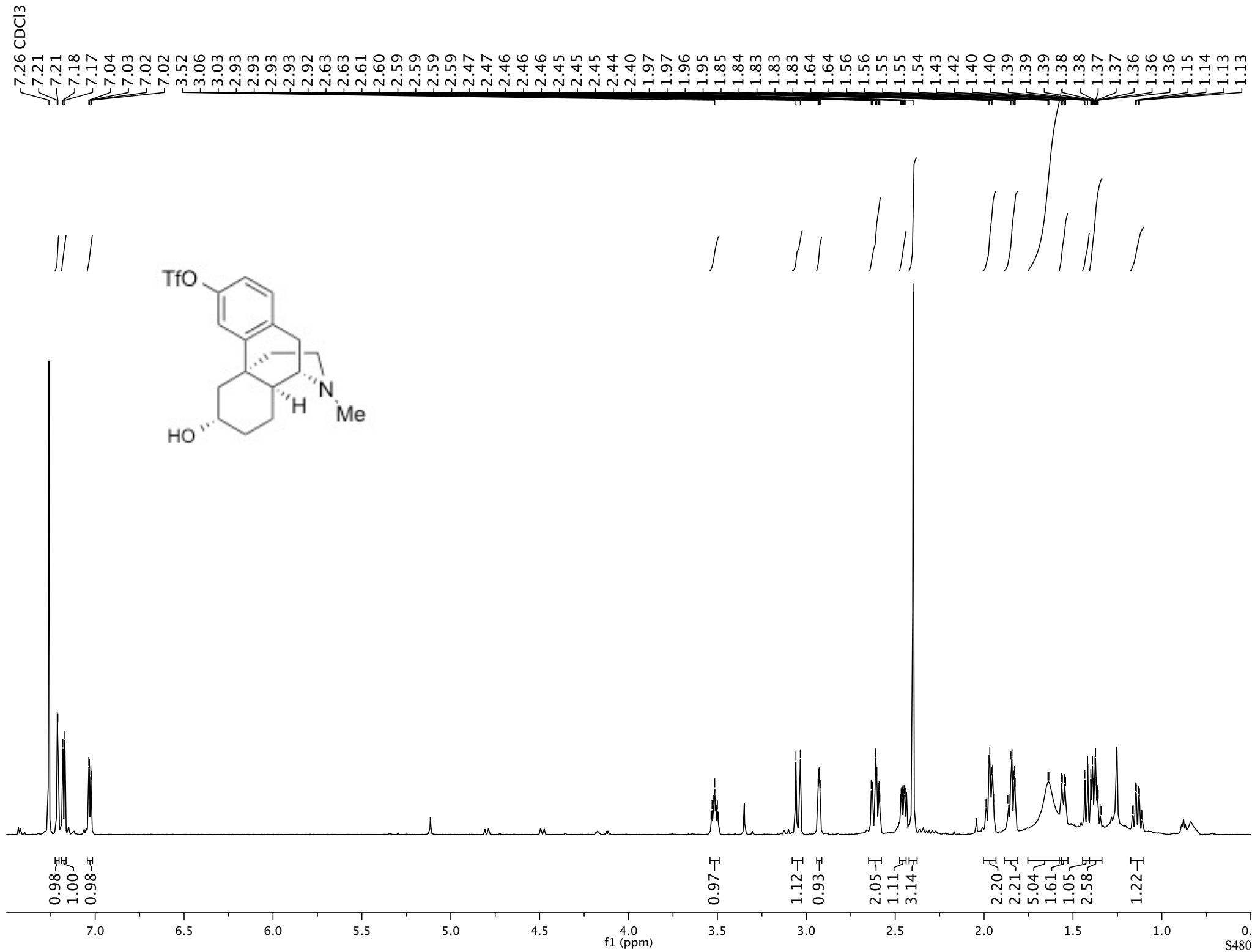




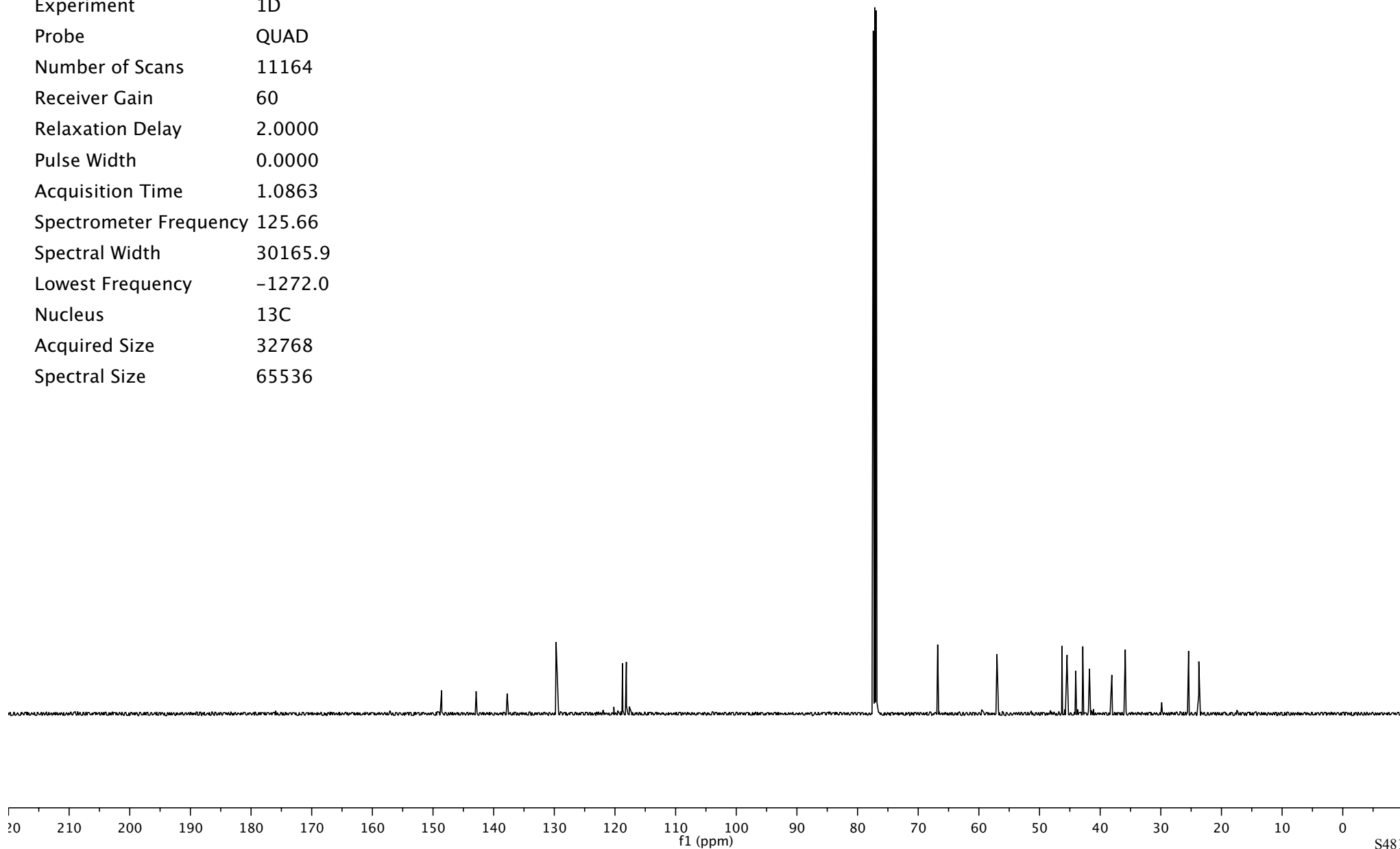
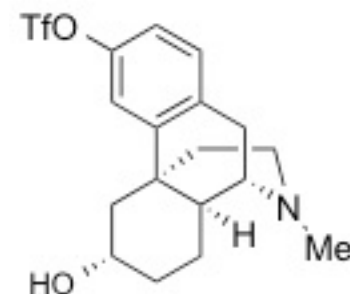
Parameter	Value
Origin	Varian
Spectrometer	vnmrs
Solvent	cdcl ₃ ⁴
Temperature	25.0
Pulse Sequence	zTOCSY1D
Experiment	1D
Probe	triax
Number of Scans	32
Receiver Gain	32
Relaxation Delay	1.5000
Pulse Width	0.0000
Acquisition Time	2.0000
Spectrometer Frequency	749.38
Spectral Width	5630.6
Lowest Frequency	369.6
Nucleus	¹ H
Acquired Size	11261
Spectral Size	65536

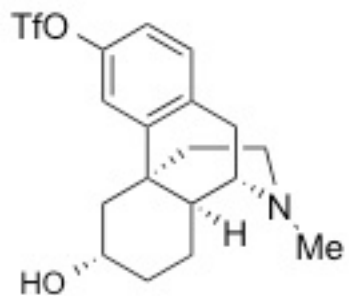
Parameter	Value
Origin	Varian
Spectrometer	vnmrs
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	triax
Number of Scans	16
Receiver Gain	32
Relaxation Delay	15.0000
Pulse Width	0.0000
Acquisition Time	2.9098
Spectrometer Frequency	749.38
Spectral Width	5630.6
Lowest Frequency	356.1
Nucleus	¹ H
Acquired Size	16384
Spectral Size	65536





Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	11164
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1272.0
Nucleus	13C
Acquired Size	32768
Spectral Size	65536





—129.71

—120.18

—118.75

—118.12

—117.63

—77.16 CDCl₃

—66.79

—57.02

—46.30

—45.45

—44.03

—42.86

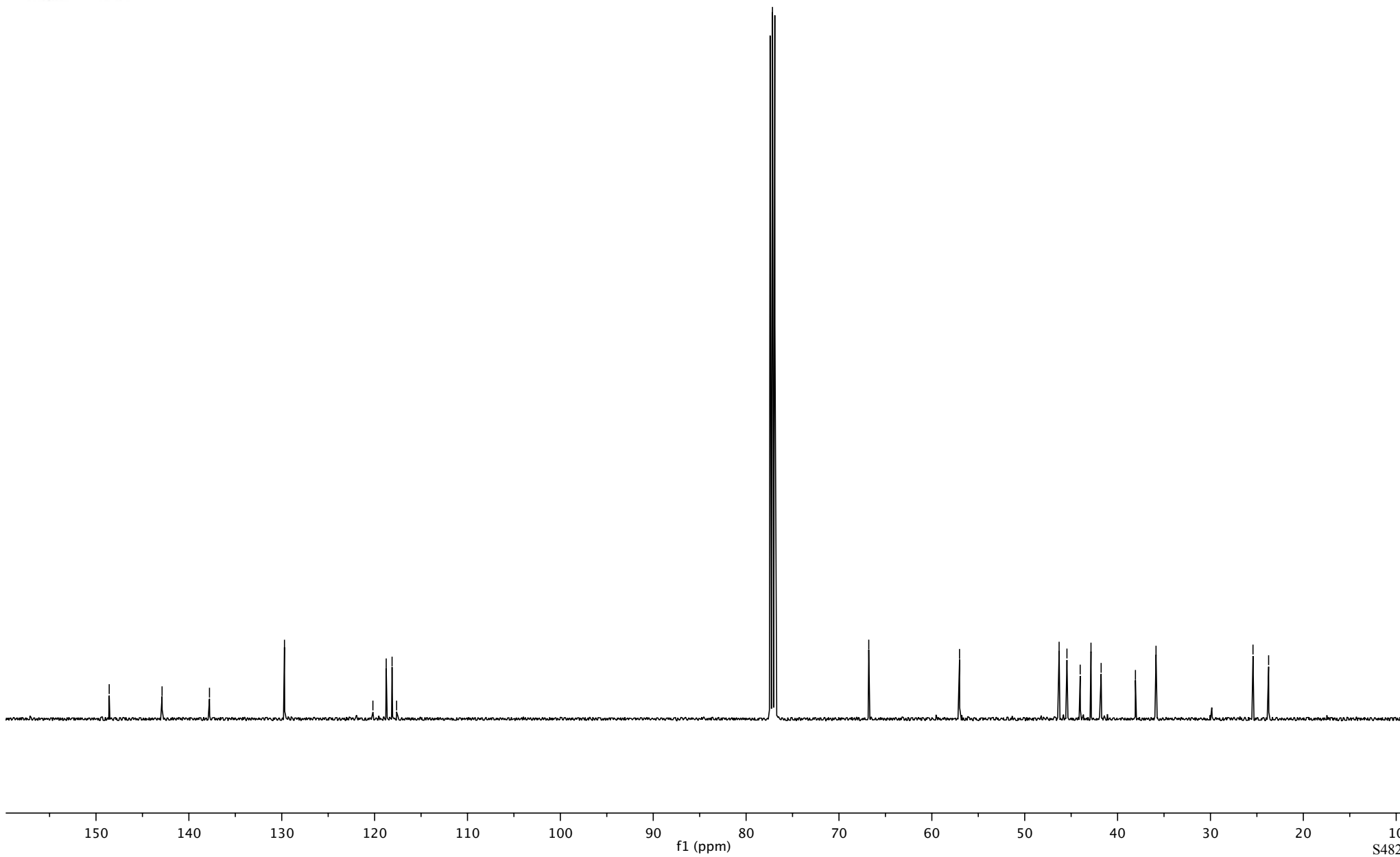
—41.77

—38.08

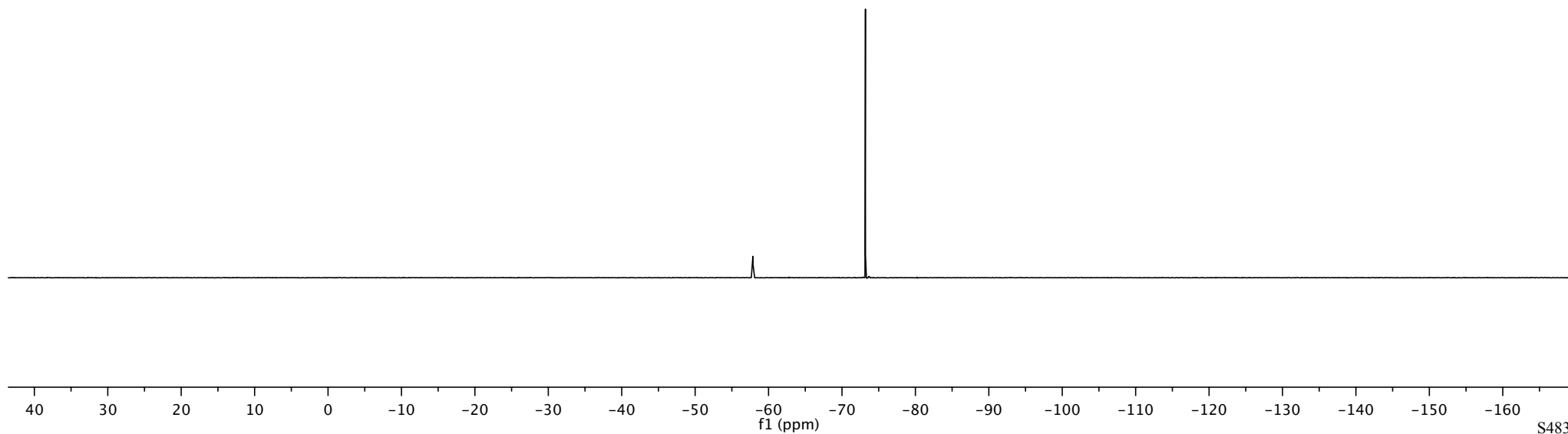
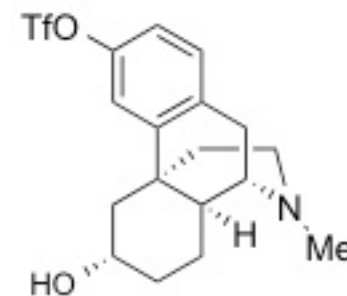
—35.86

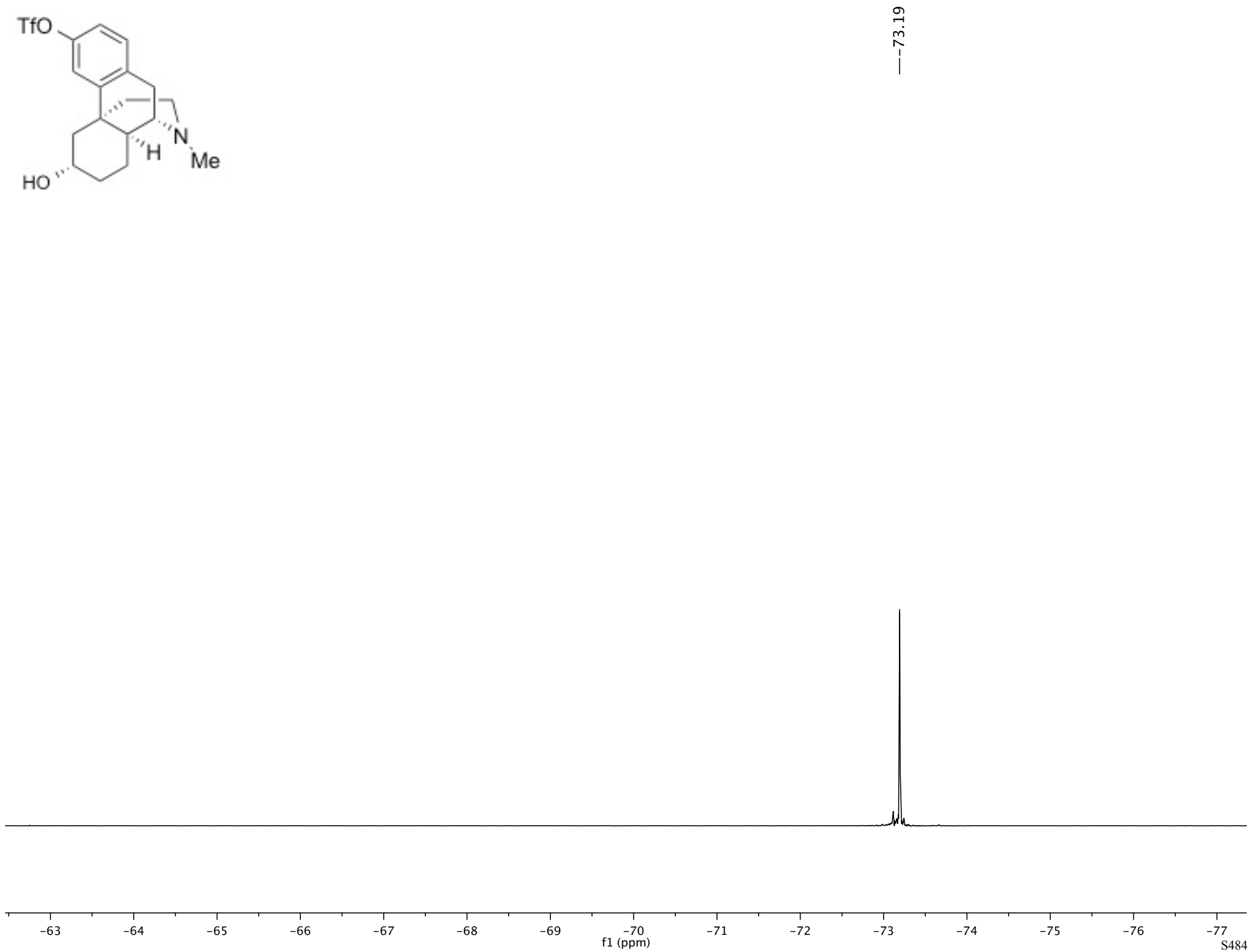
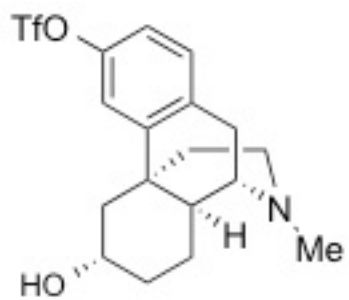
—25.42

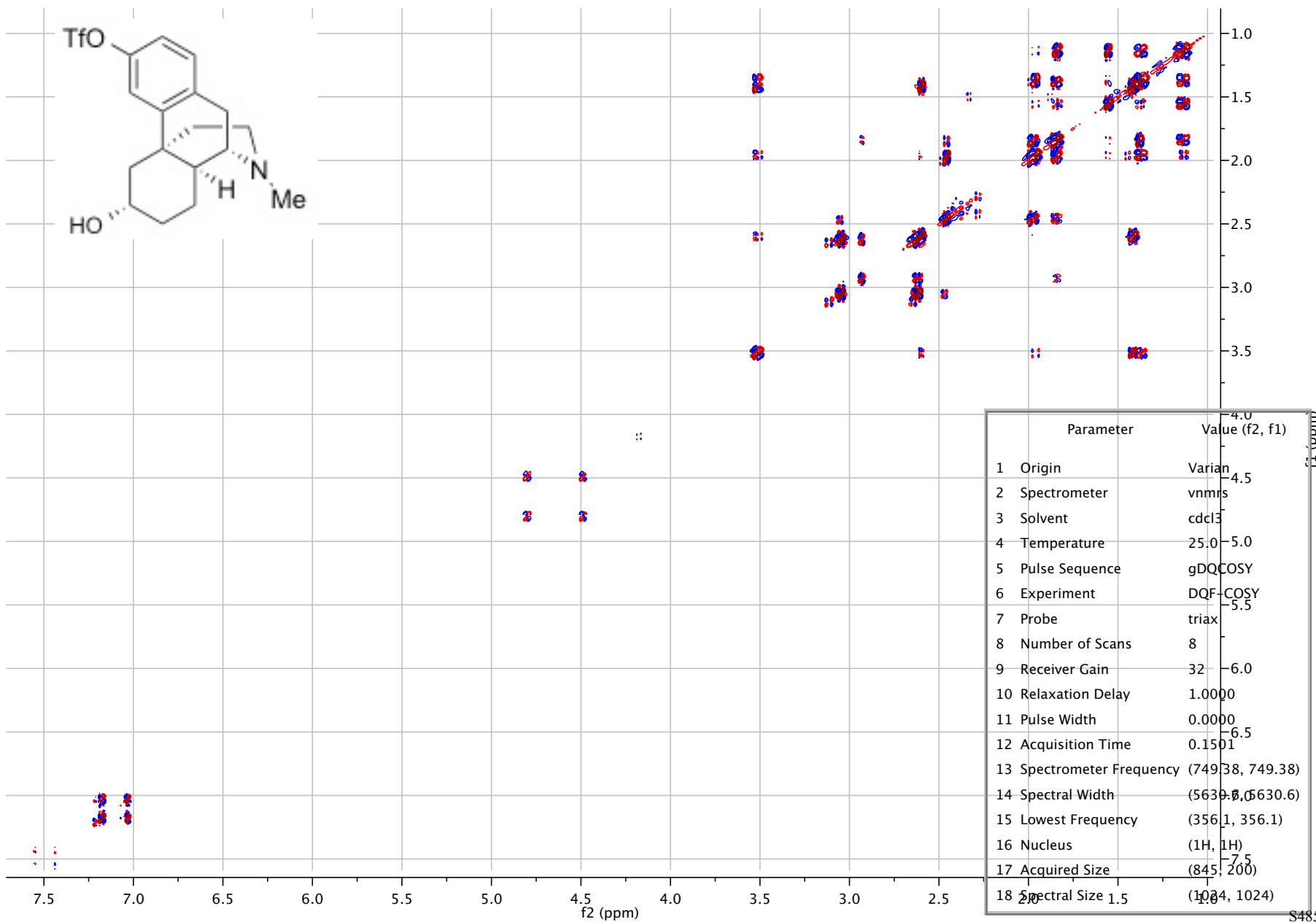
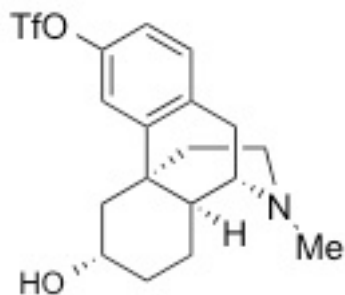
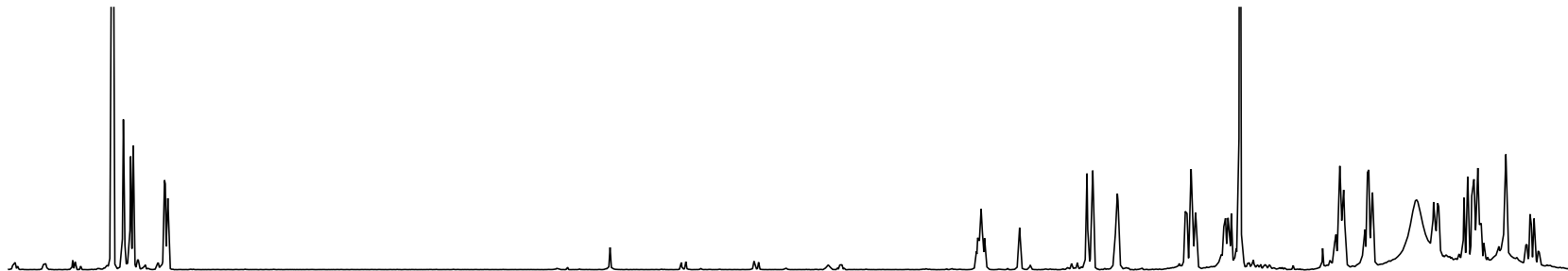
—23.74



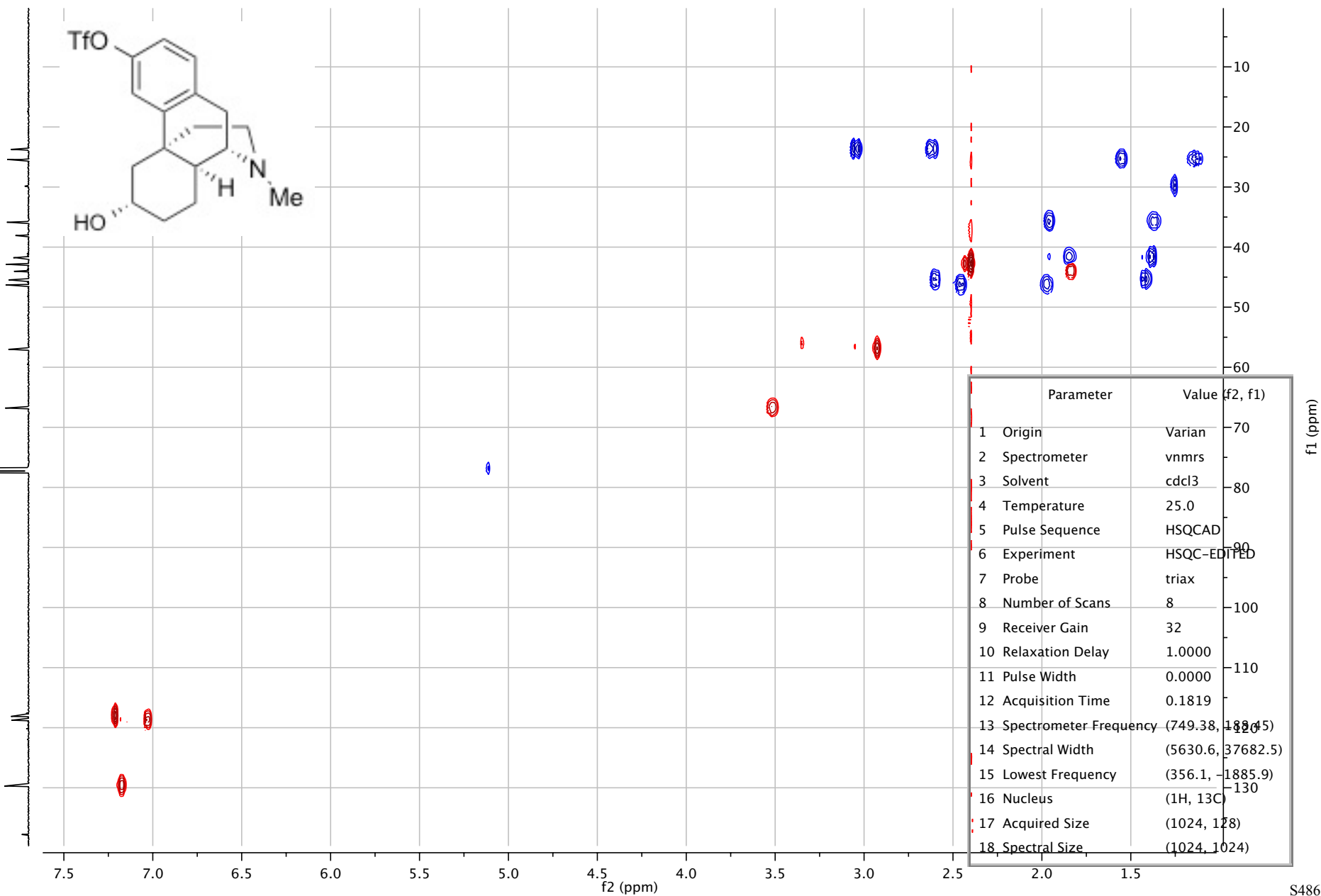
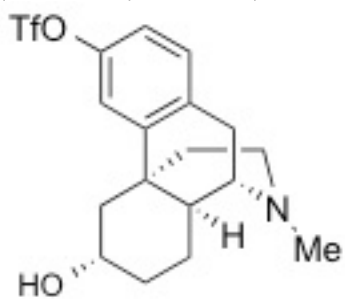
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	128
Receiver Gain	50
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency	-79501.3
Nucleus	¹⁹ F
Acquired Size	32768
Spectral Size	65536

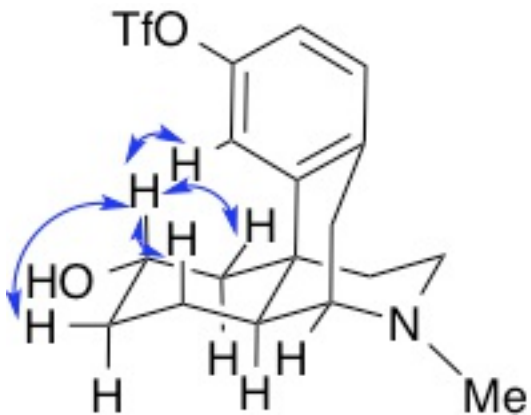




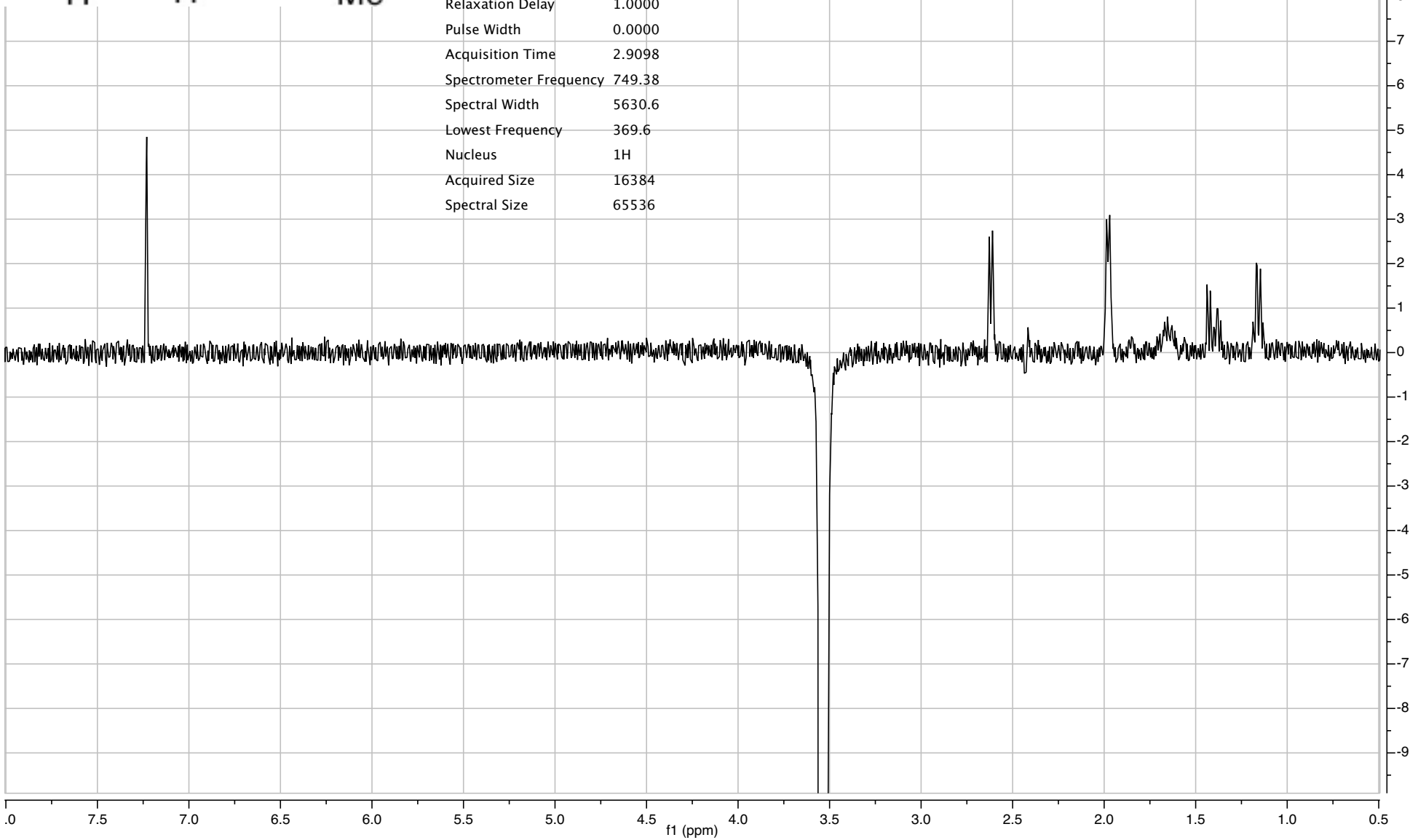


Parameter		Value (f2, f1)
1	Origin	Varian
2	Spectrometer	vnmr1s
3	Solvent	cdcl3
4	Temperature	25.0
5	Pulse Sequence	gDQF-COSY
6	Experiment	DQF-COSY
7	Probe	triax
8	Number of Scans	8
9	Receiver Gain	32
10	Relaxation Delay	1.0000
11	Pulse Width	0.0000
12	Acquisition Time	0.1501
13	Spectrometer Frequency	(749.138, 749.38)
14	Spectral Width	(5639.0, 5630.6)
15	Lowest Frequency	(356.1, 356.1)
16	Nucleus	(1H, 1H)
17	Acquired Size	(845, 200)
18	Spectral Size	(1024, 1024)

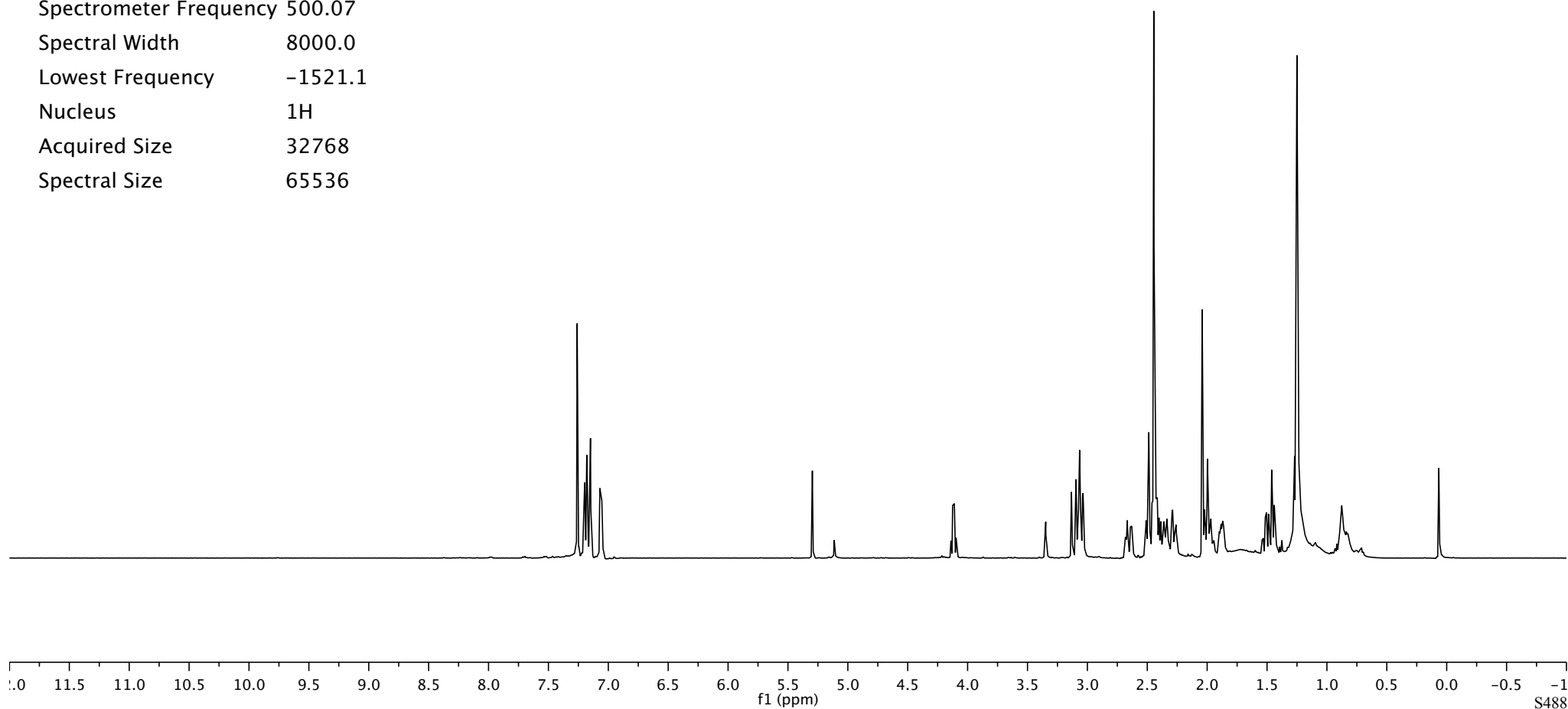
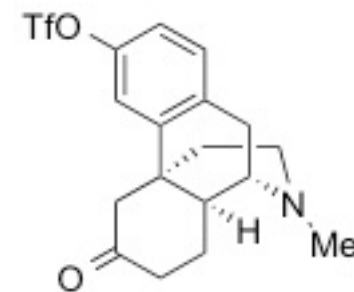


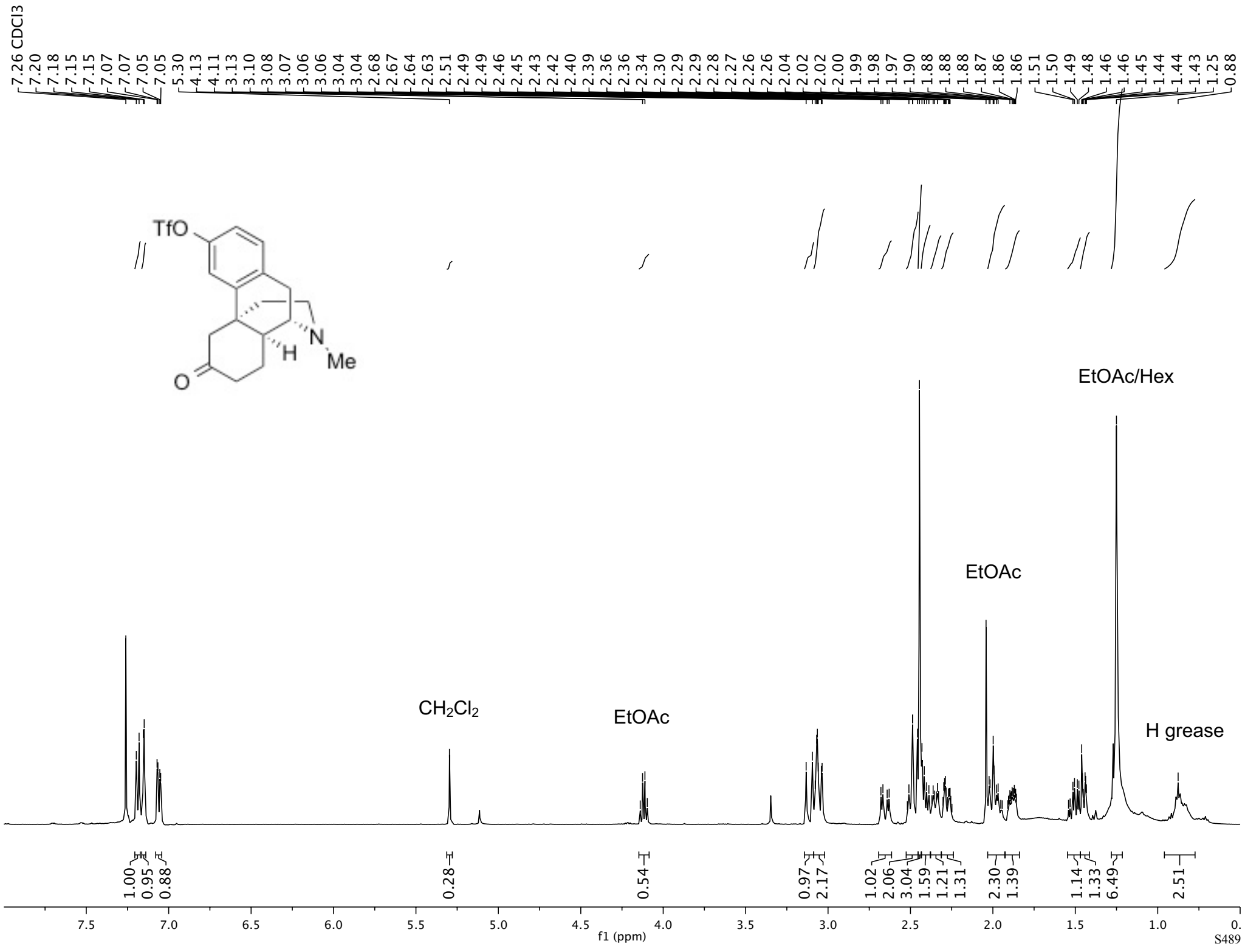
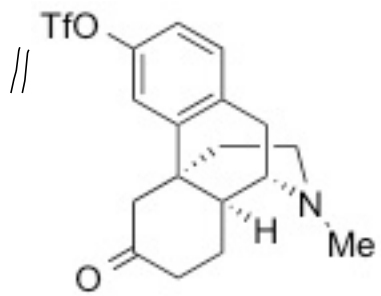


Parameter	Value
Origin	Varian
Spectrometer	vnmrs
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	NOESY1D
Experiment	1D-NOESY
Probe	triax
Number of Scans	128
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	2.9098
Spectrometer Frequency	749.38
Spectral Width	5630.6
Lowest Frequency	369.6
Nucleus	¹ H
Acquired Size	16384
Spectral Size	65536

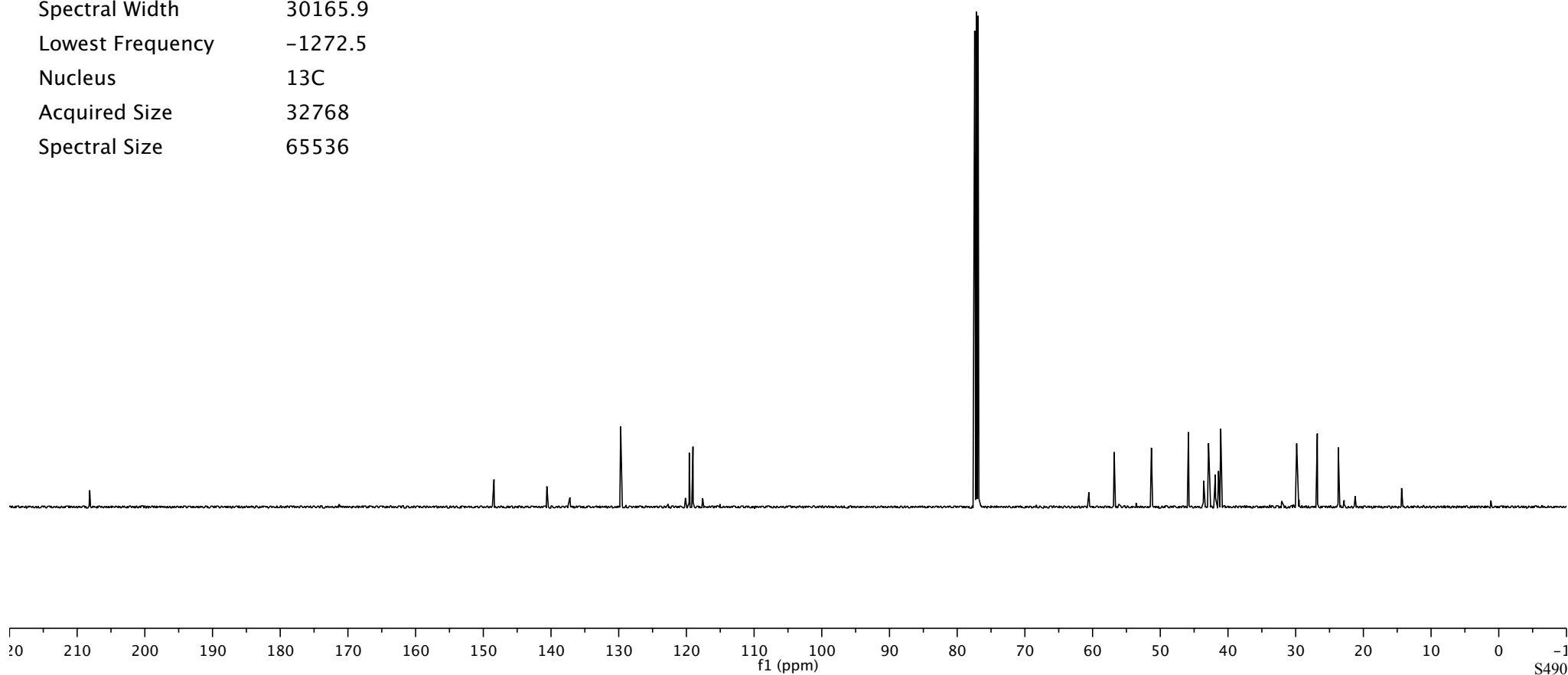
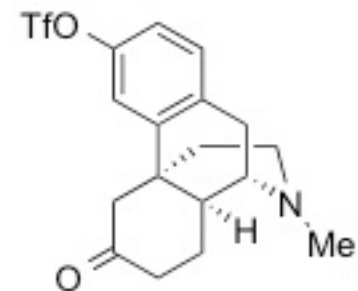


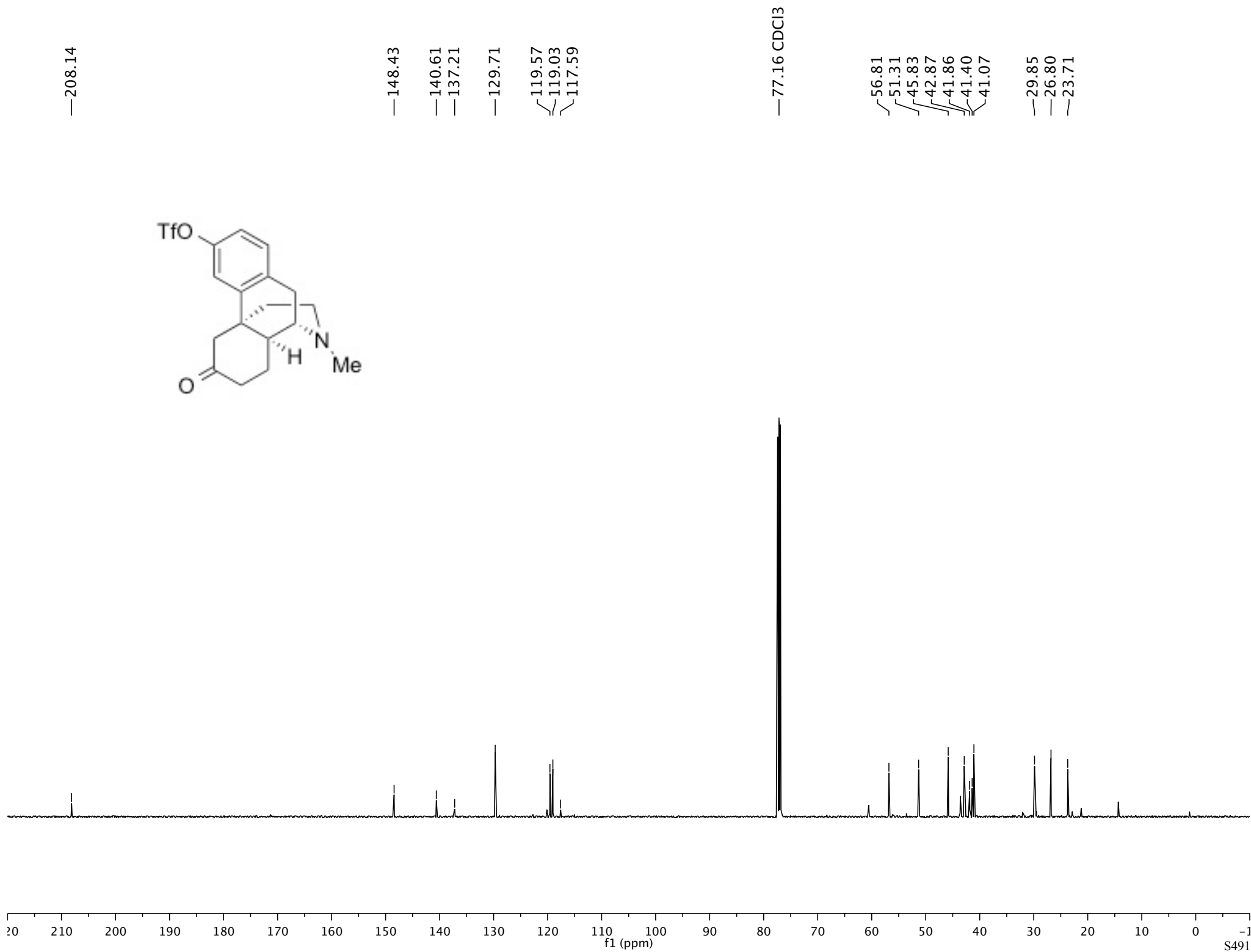
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	50.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	32
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

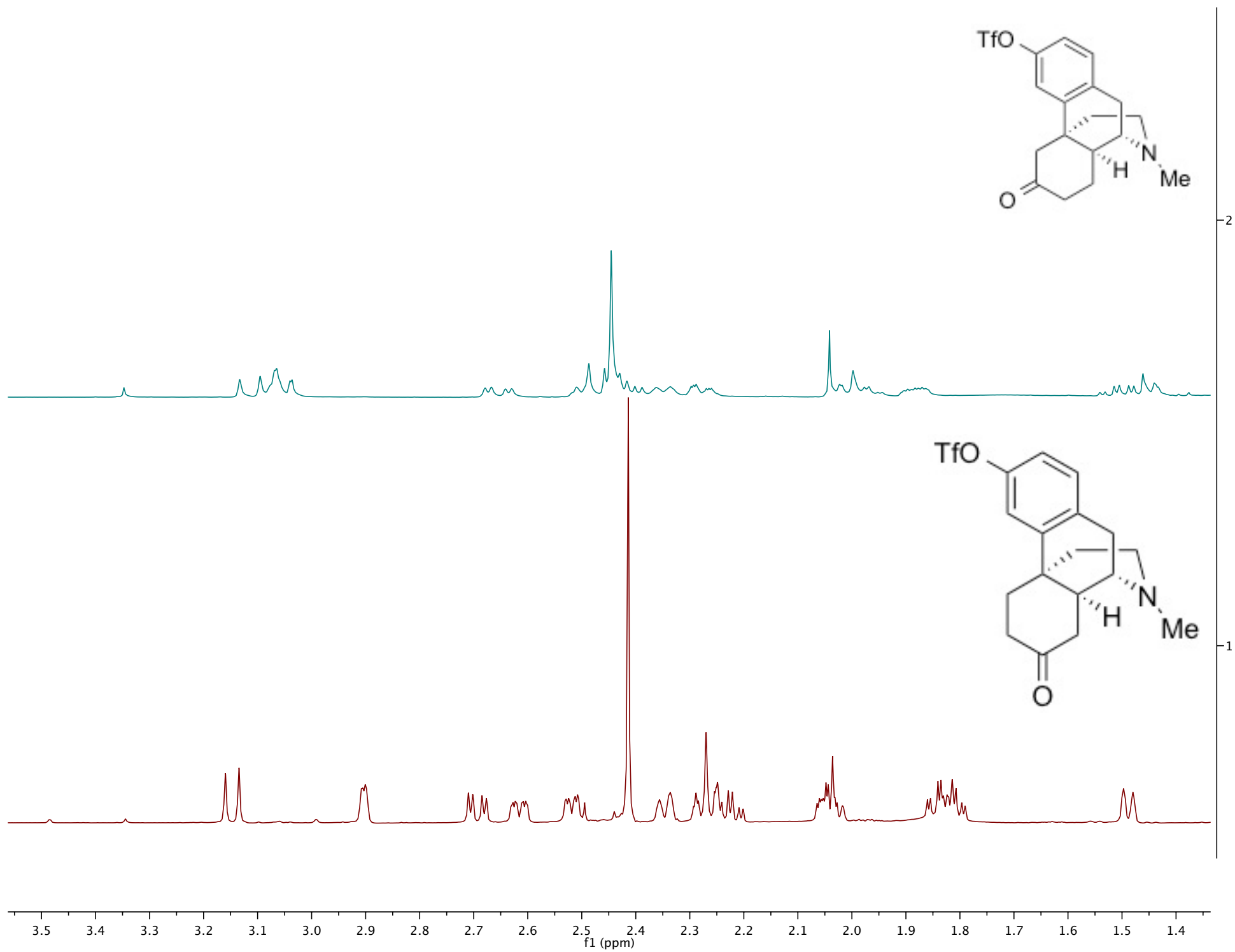




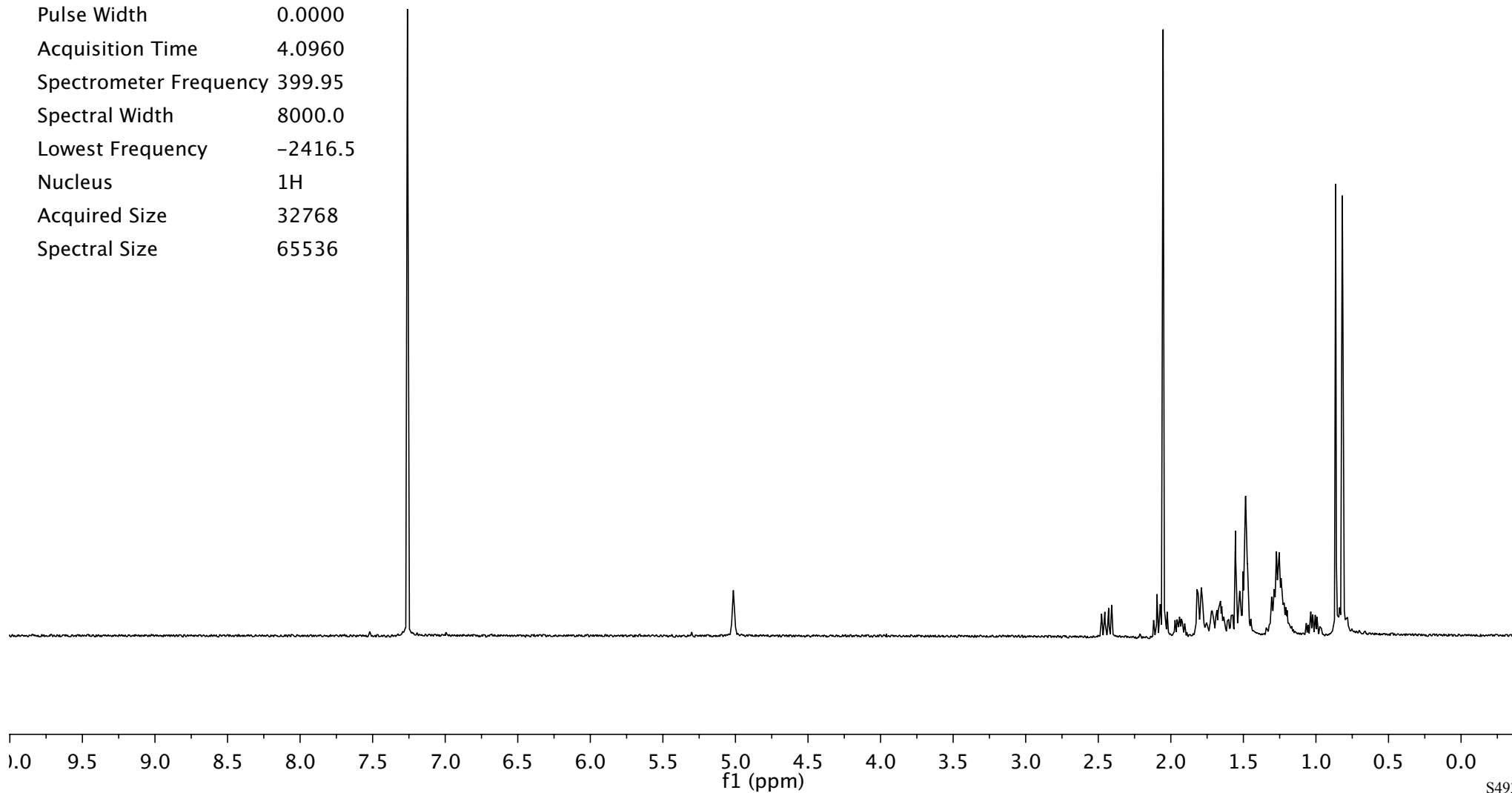
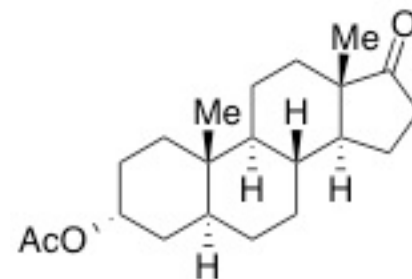
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	50.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	14167
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1272.5
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

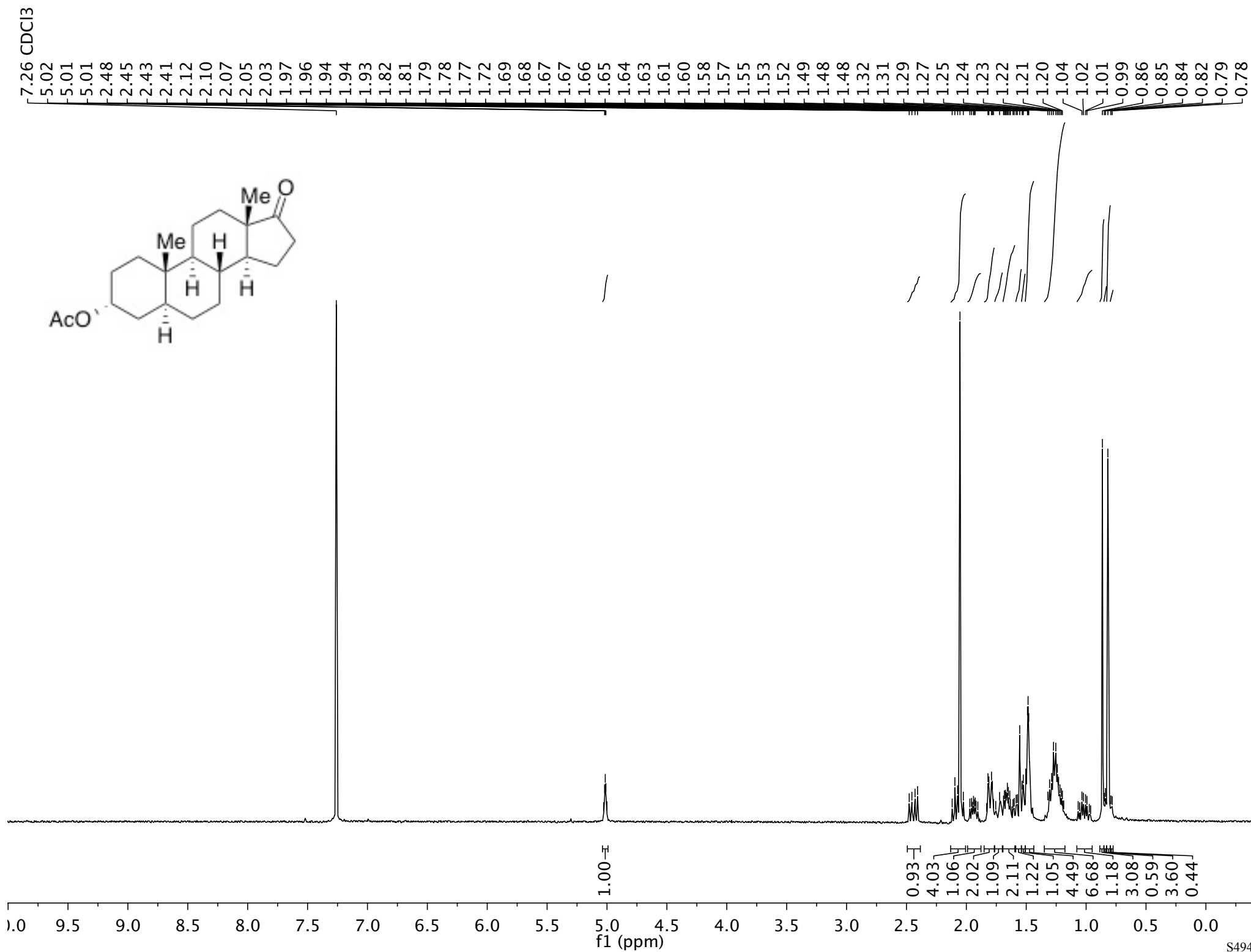




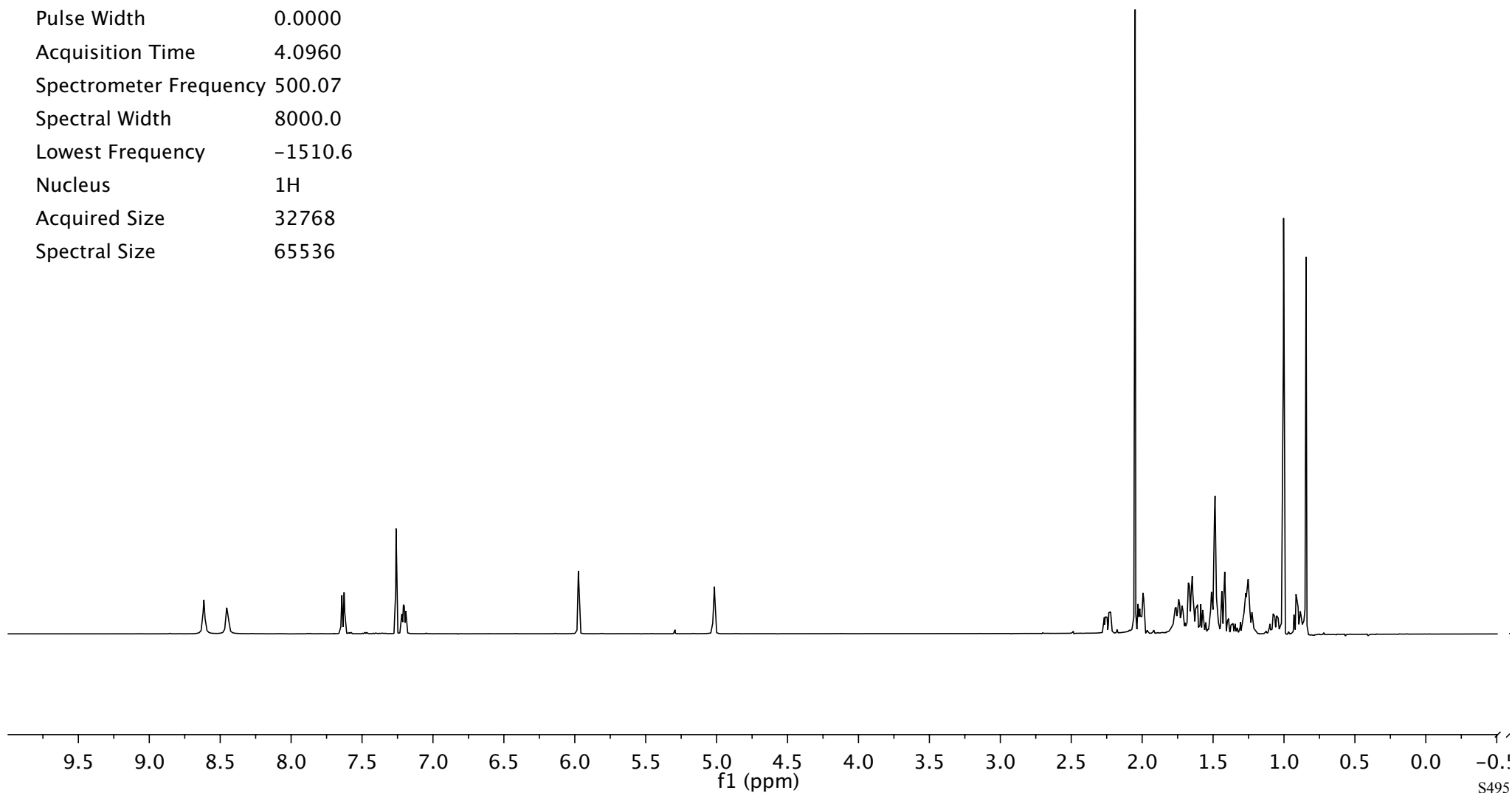
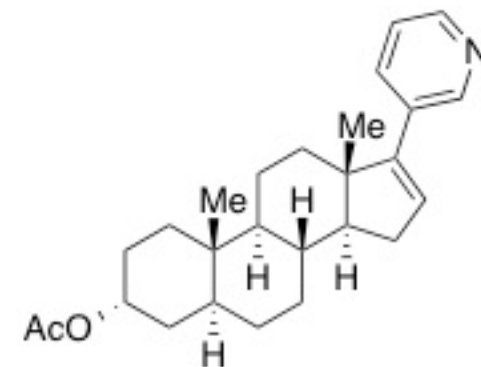


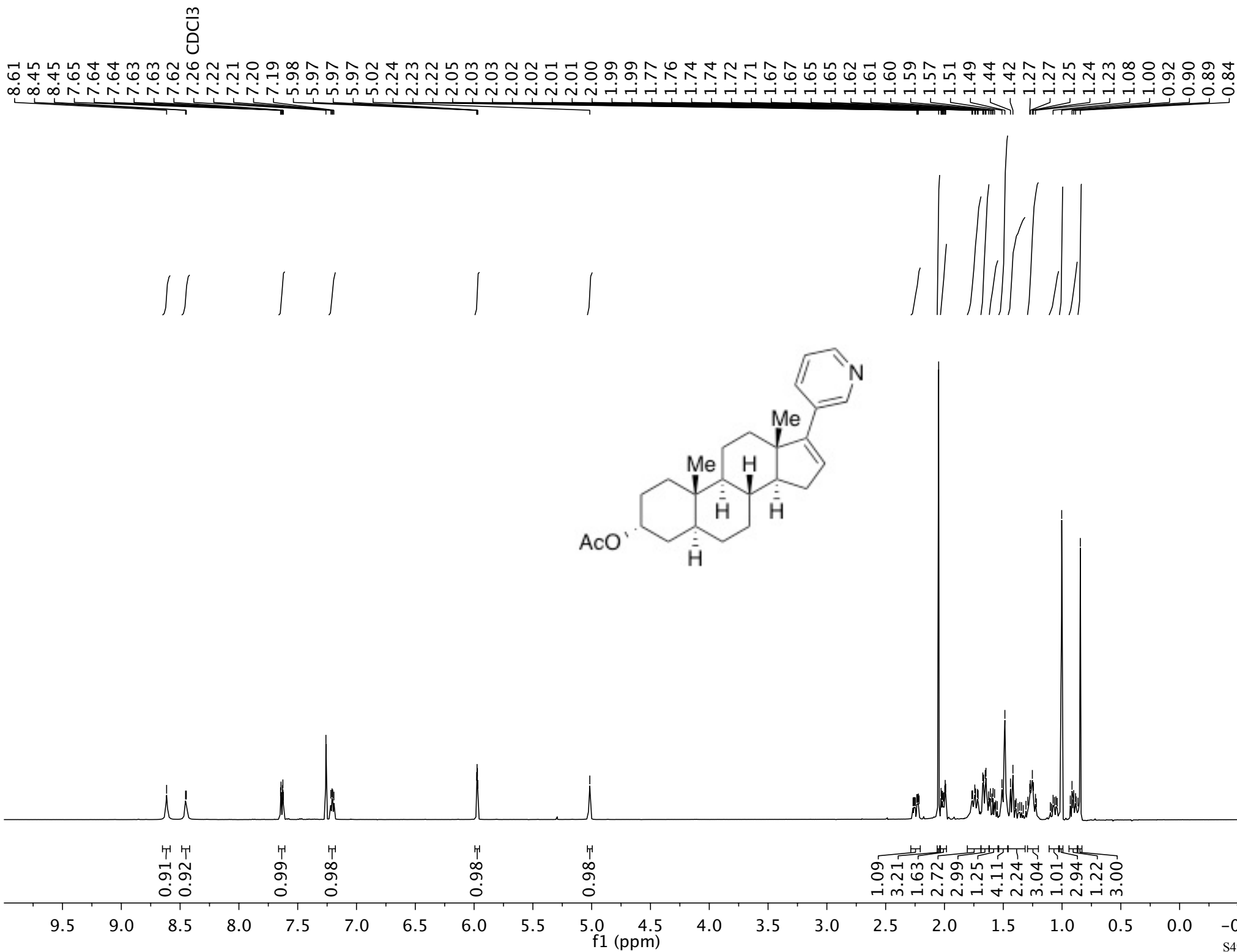
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	399.95
Spectral Width	8000.0
Lowest Frequency	-2416.5
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



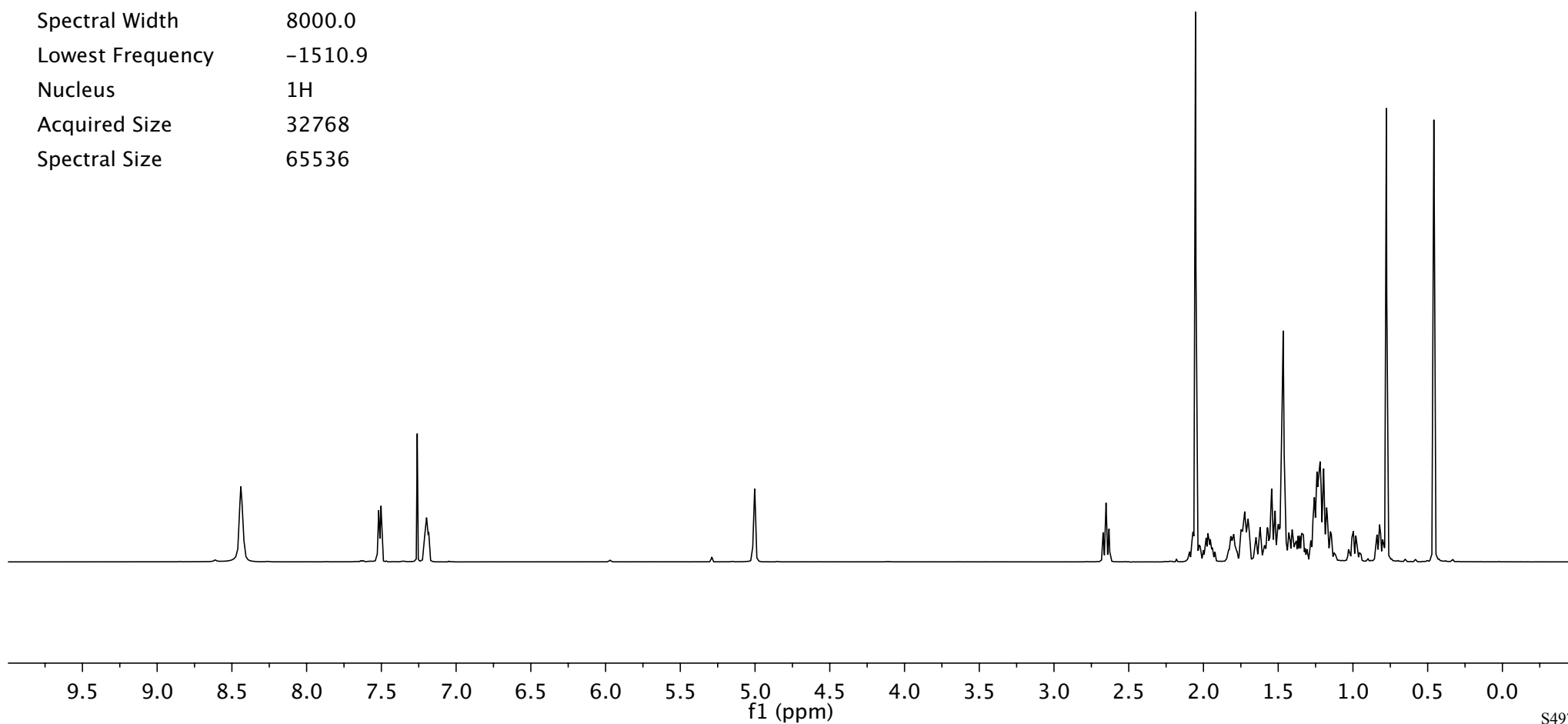
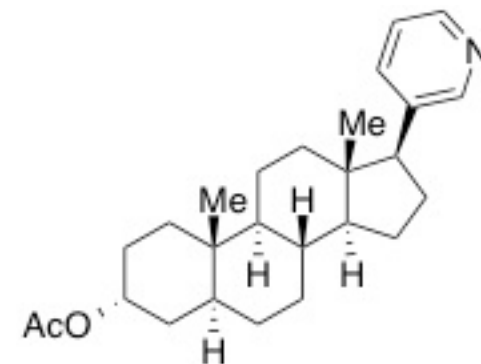


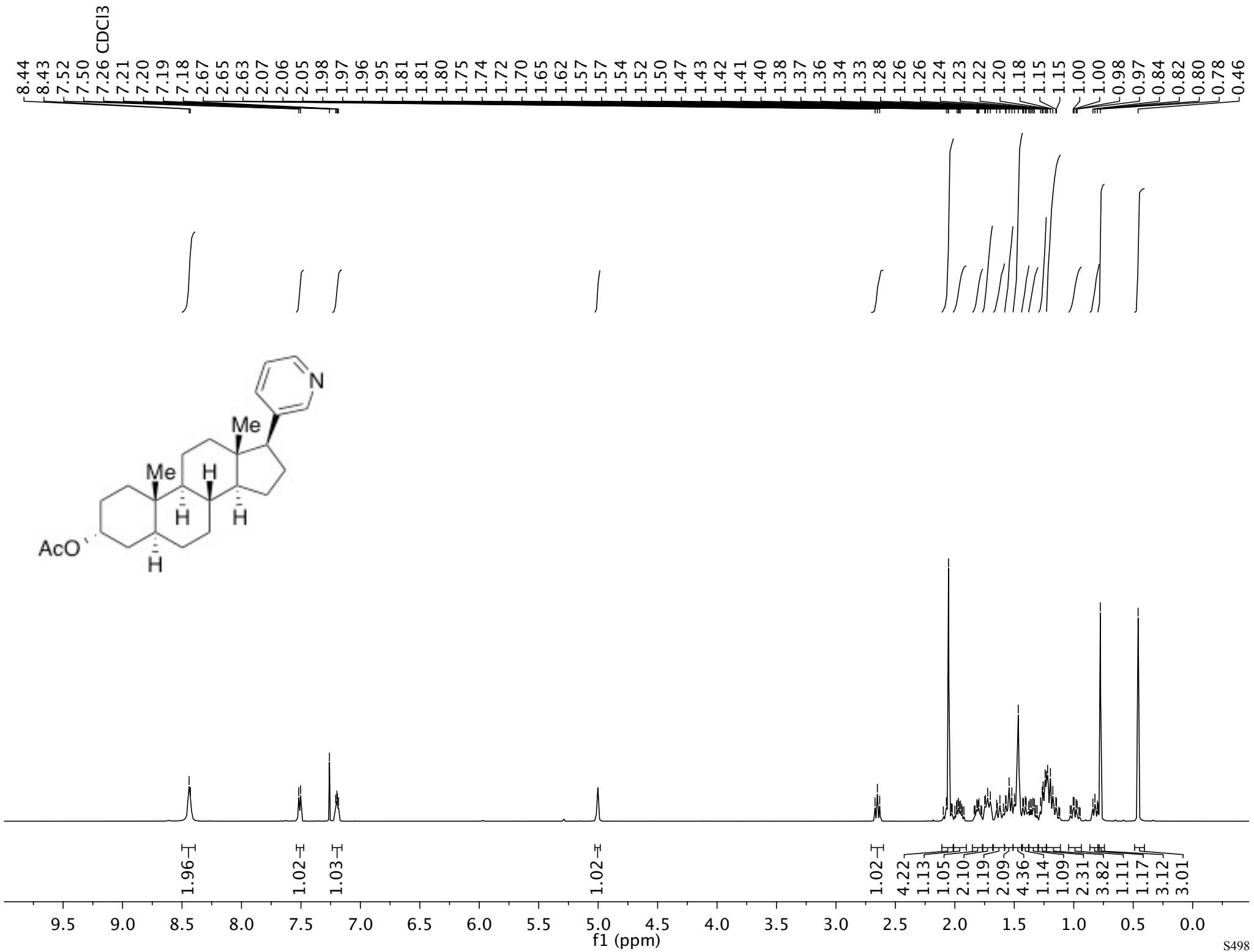
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	30
Relaxation Delay	15.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1510.6
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



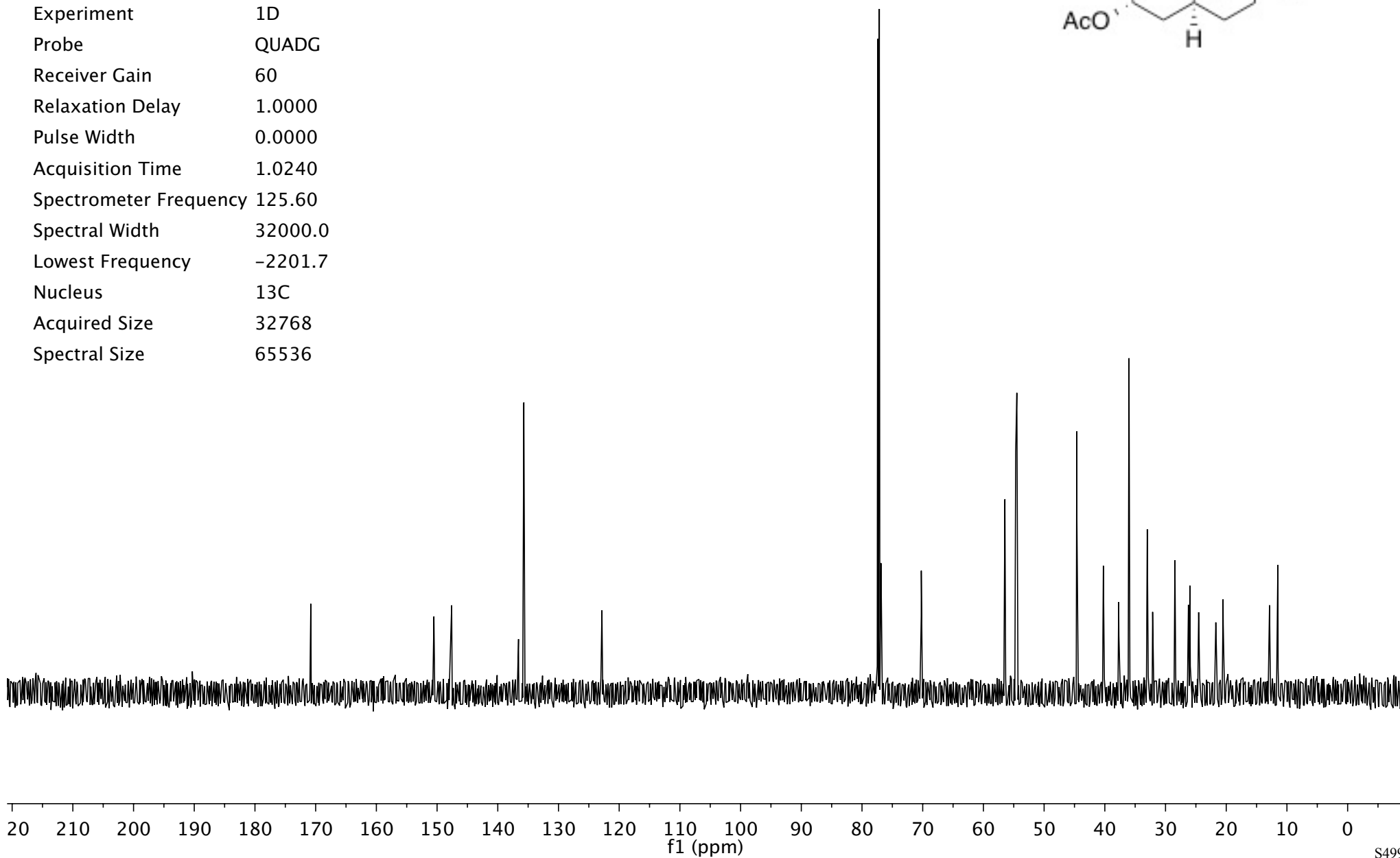
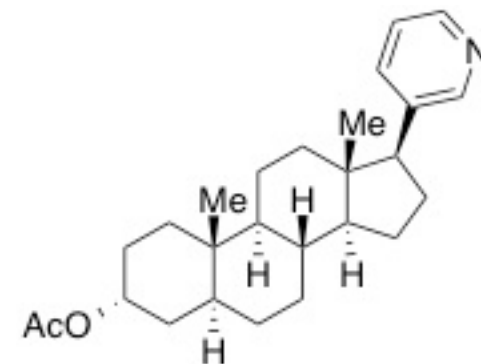


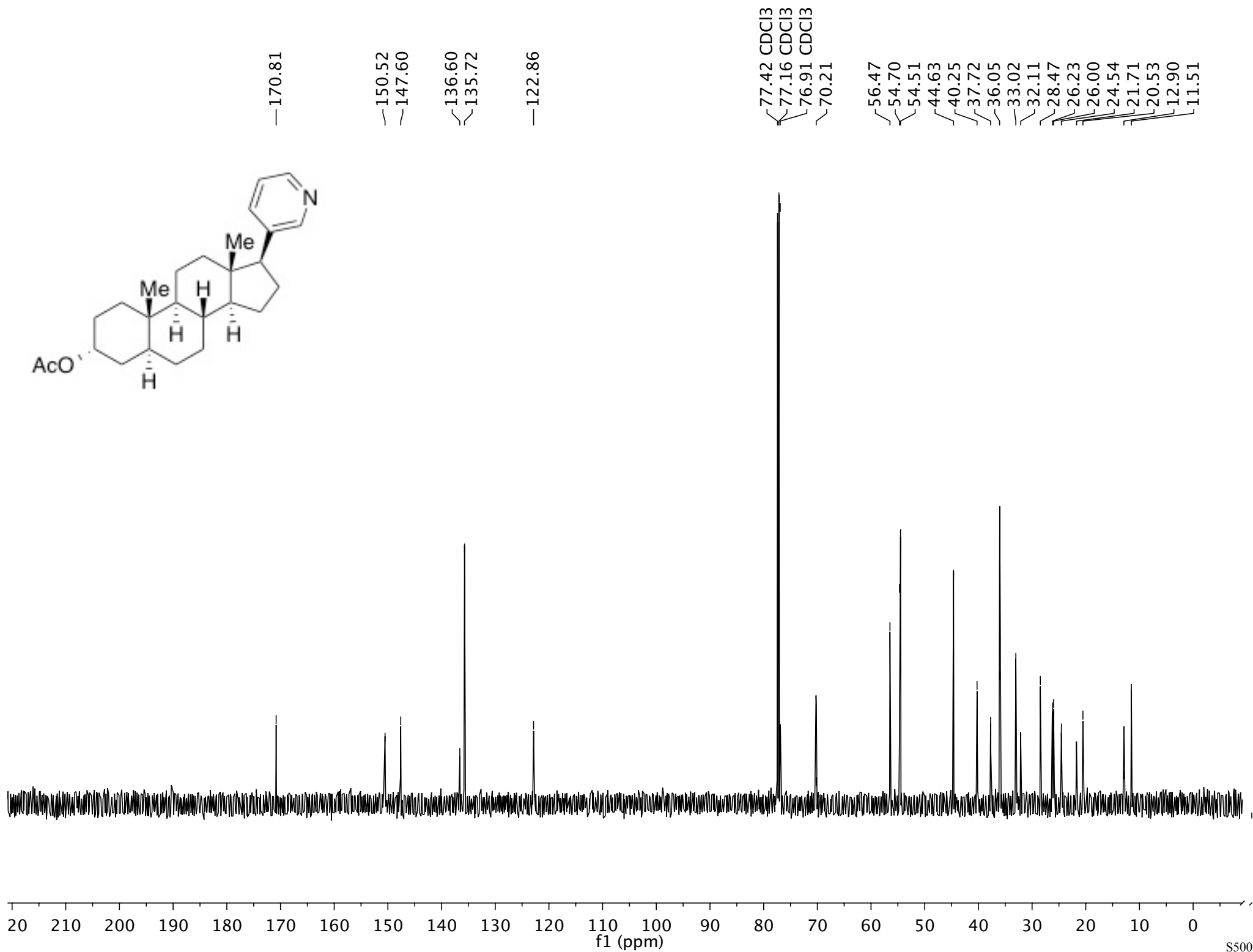
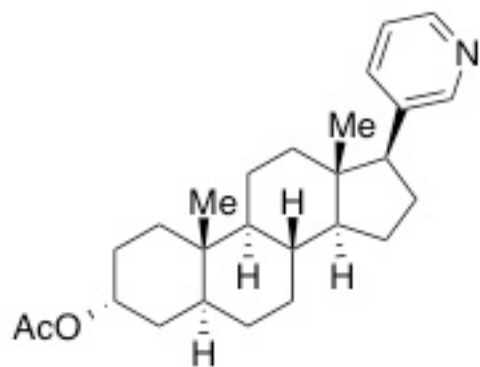
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	32
Relaxation Delay	15.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1510.9
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

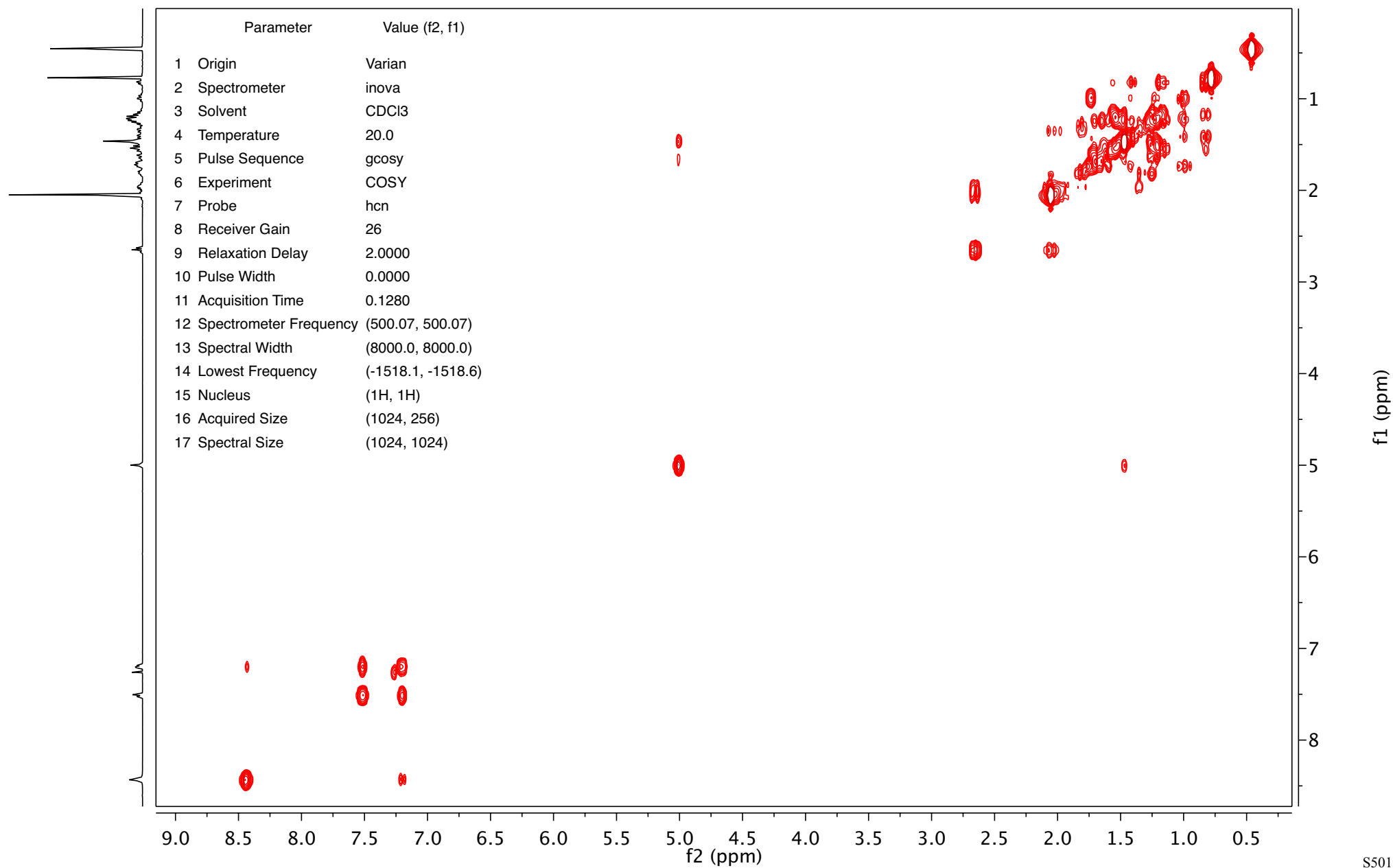
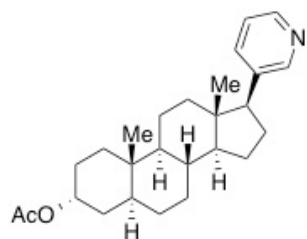


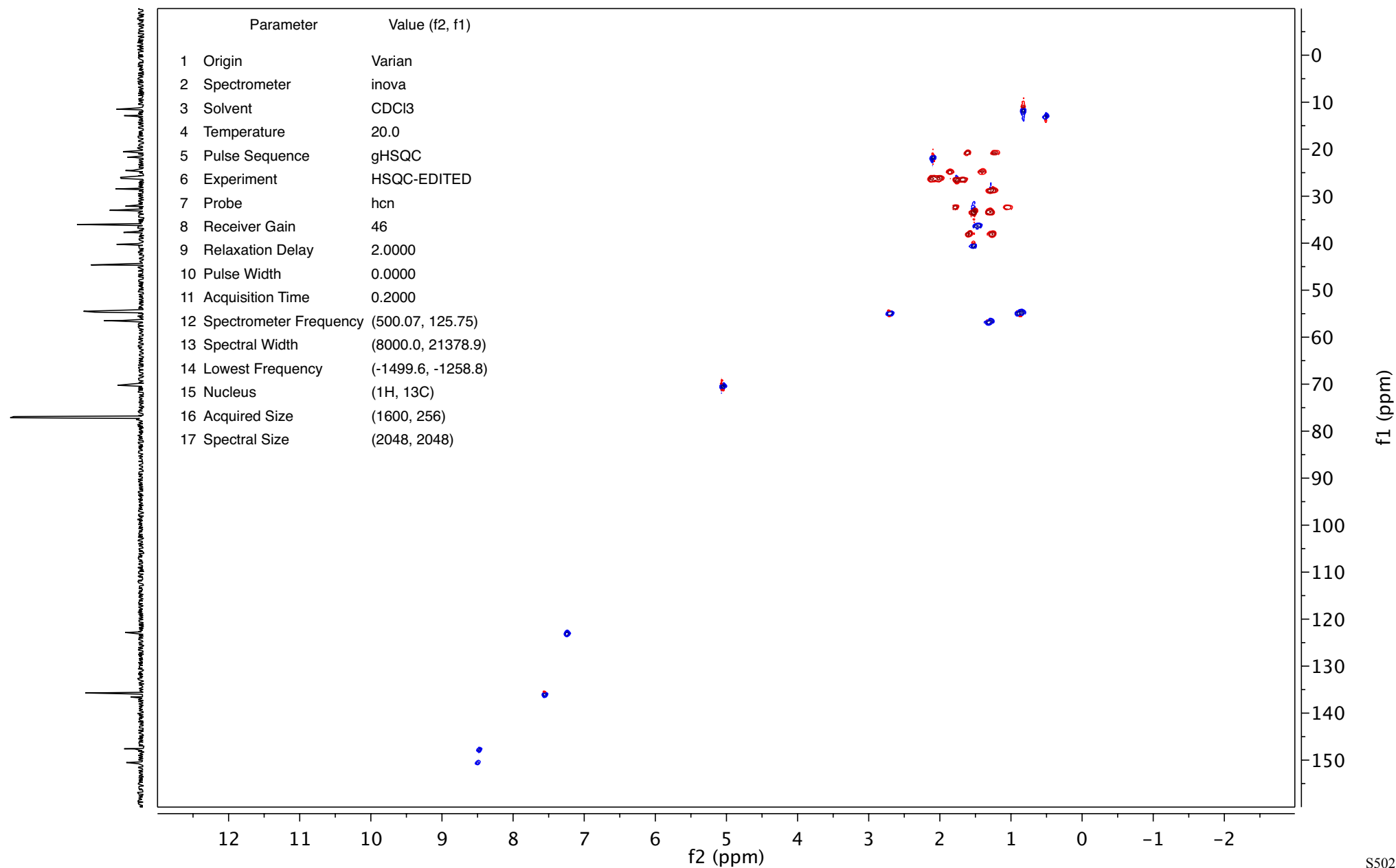
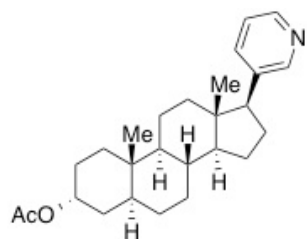


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2201.7
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

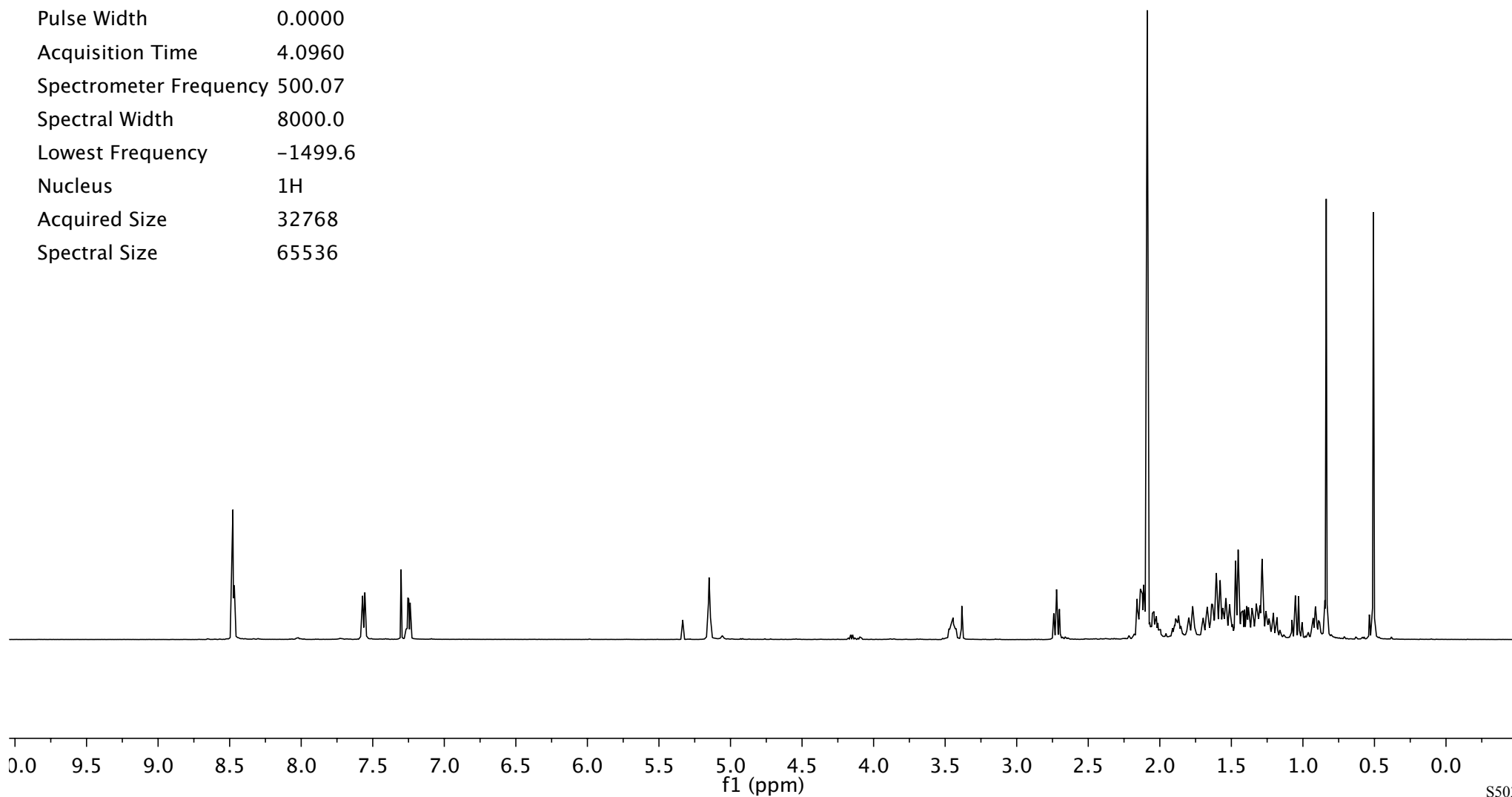
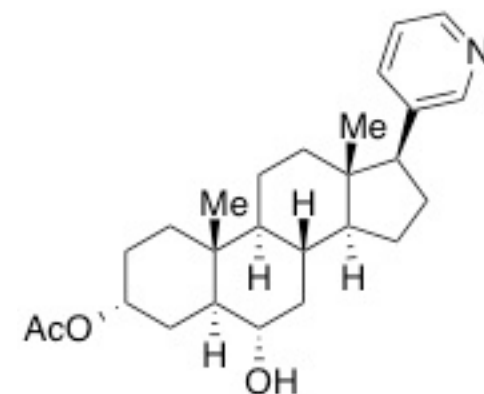


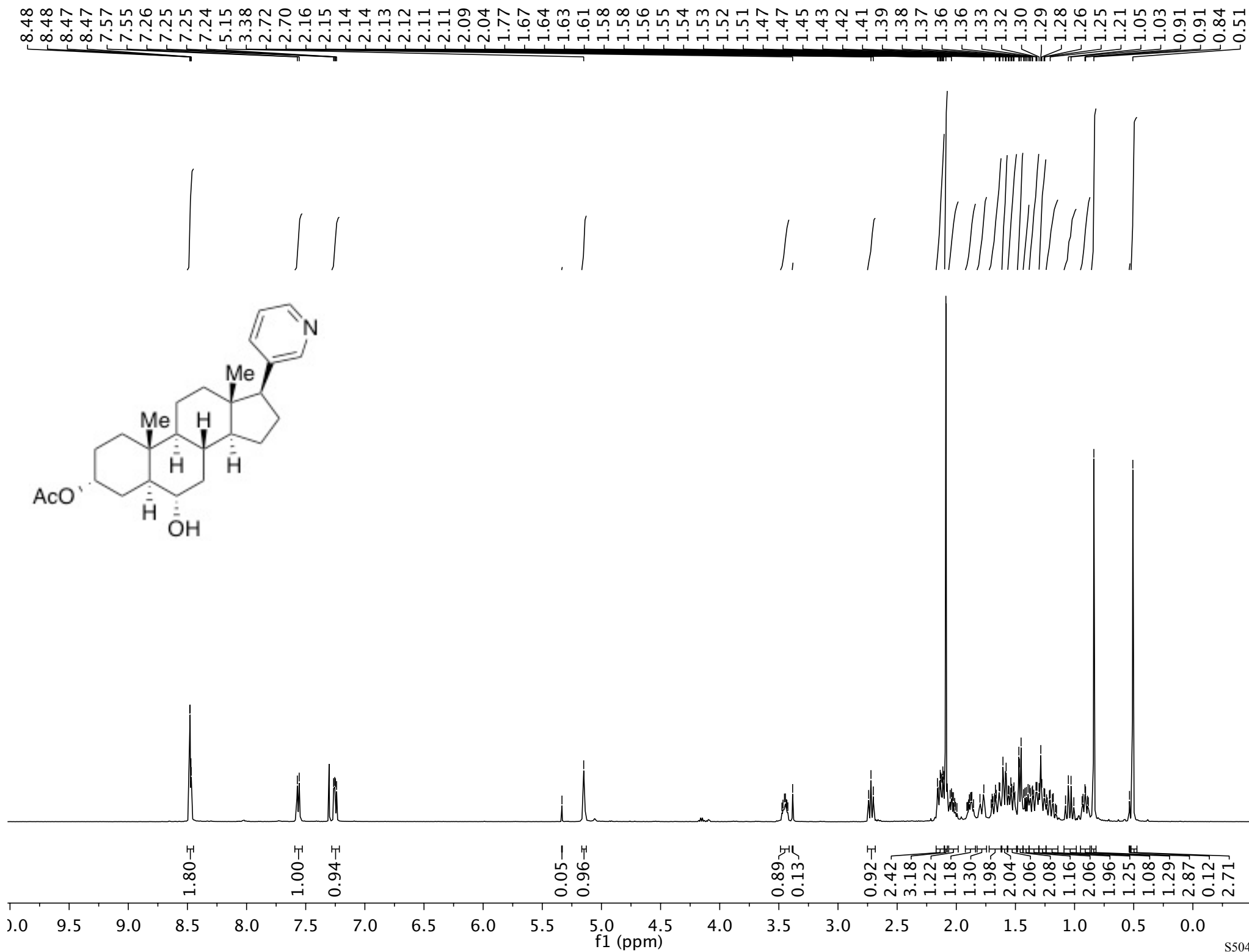




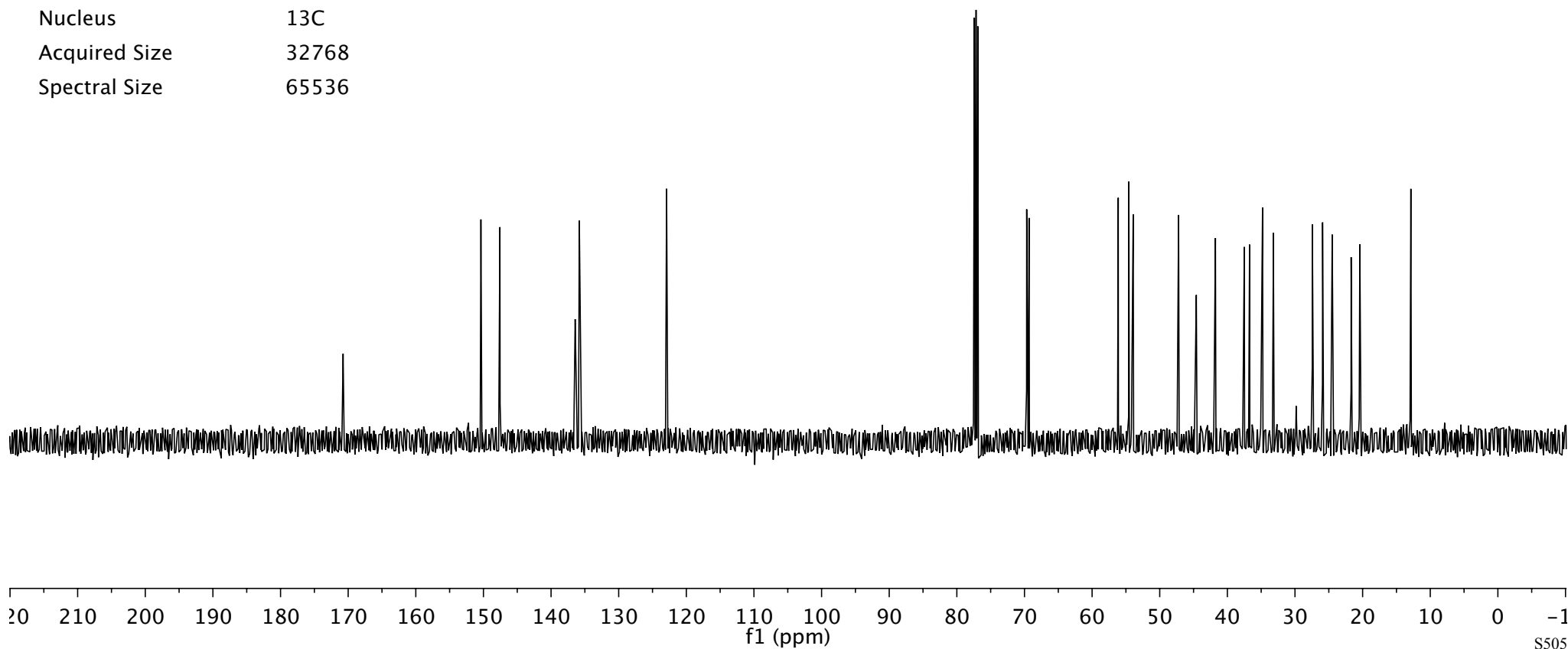
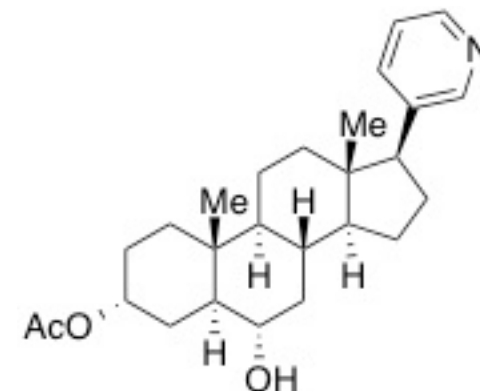


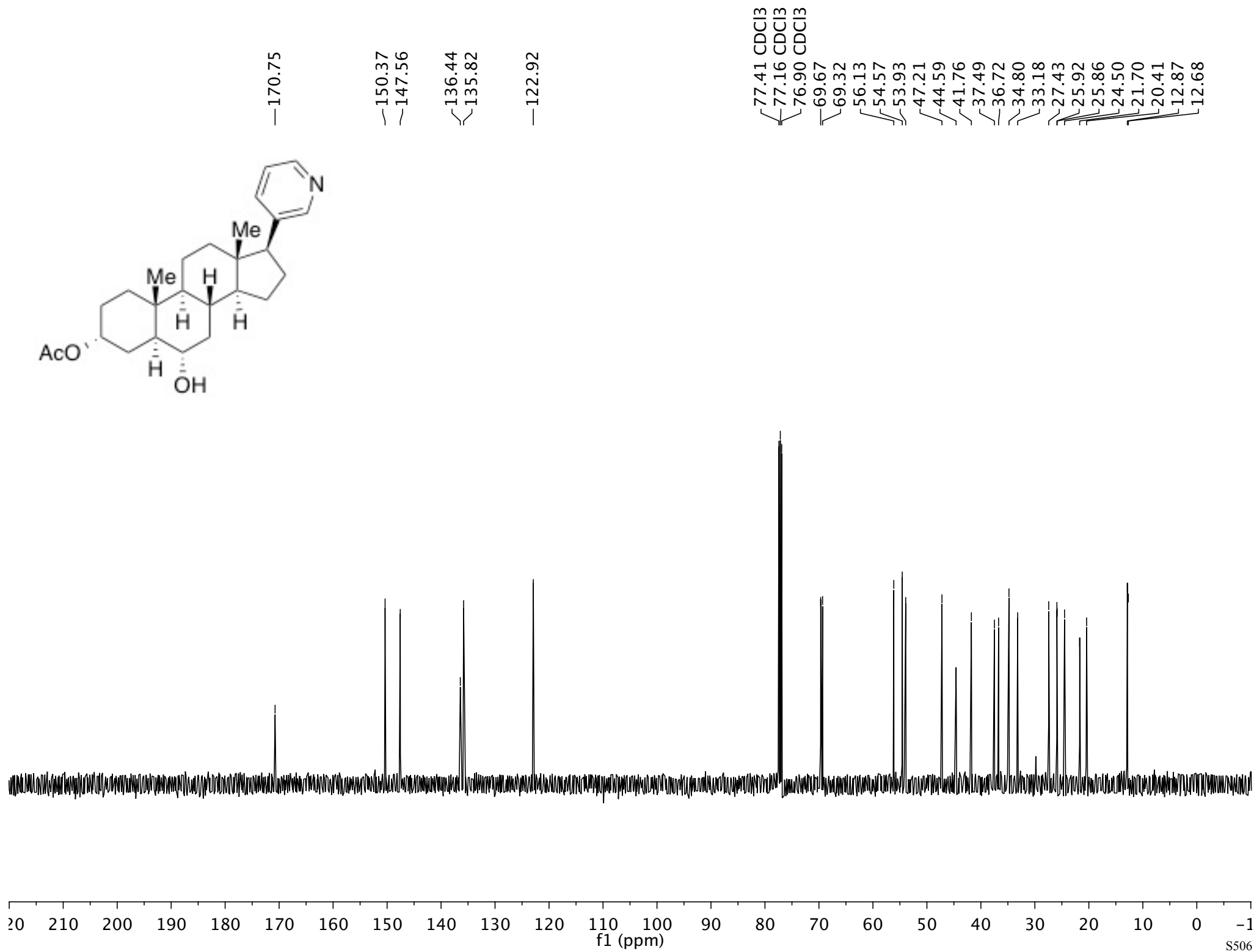
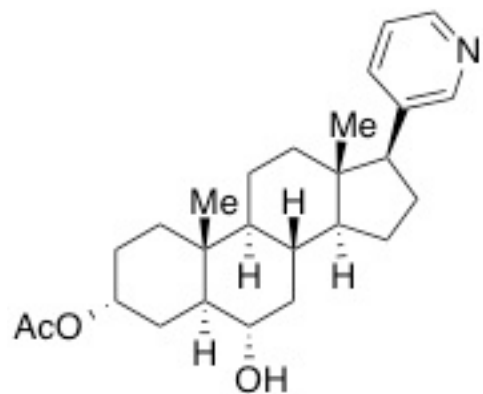
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	32
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1499.6
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

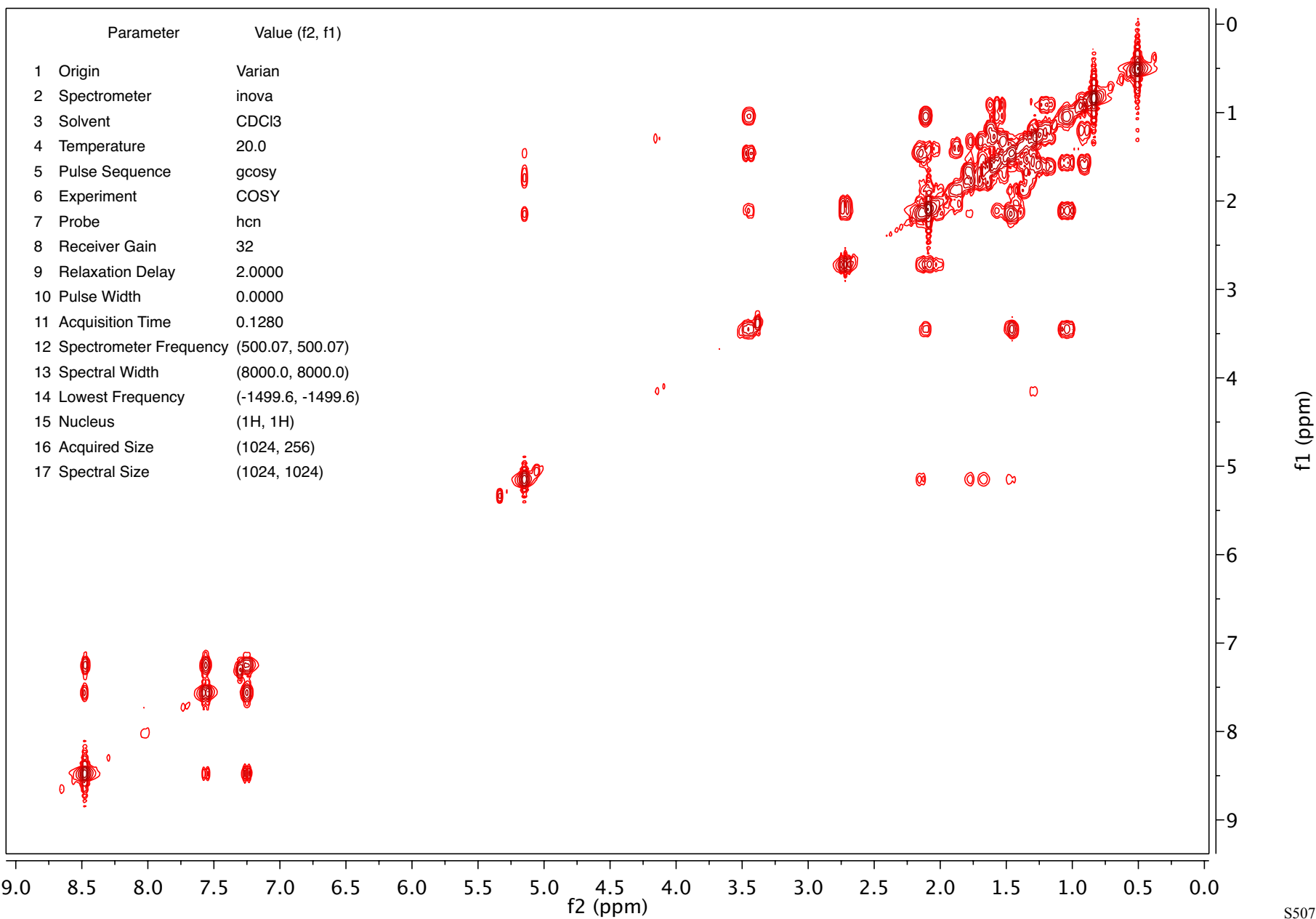
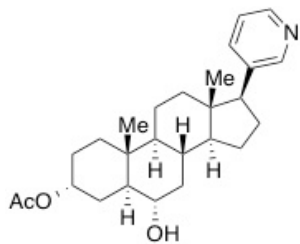


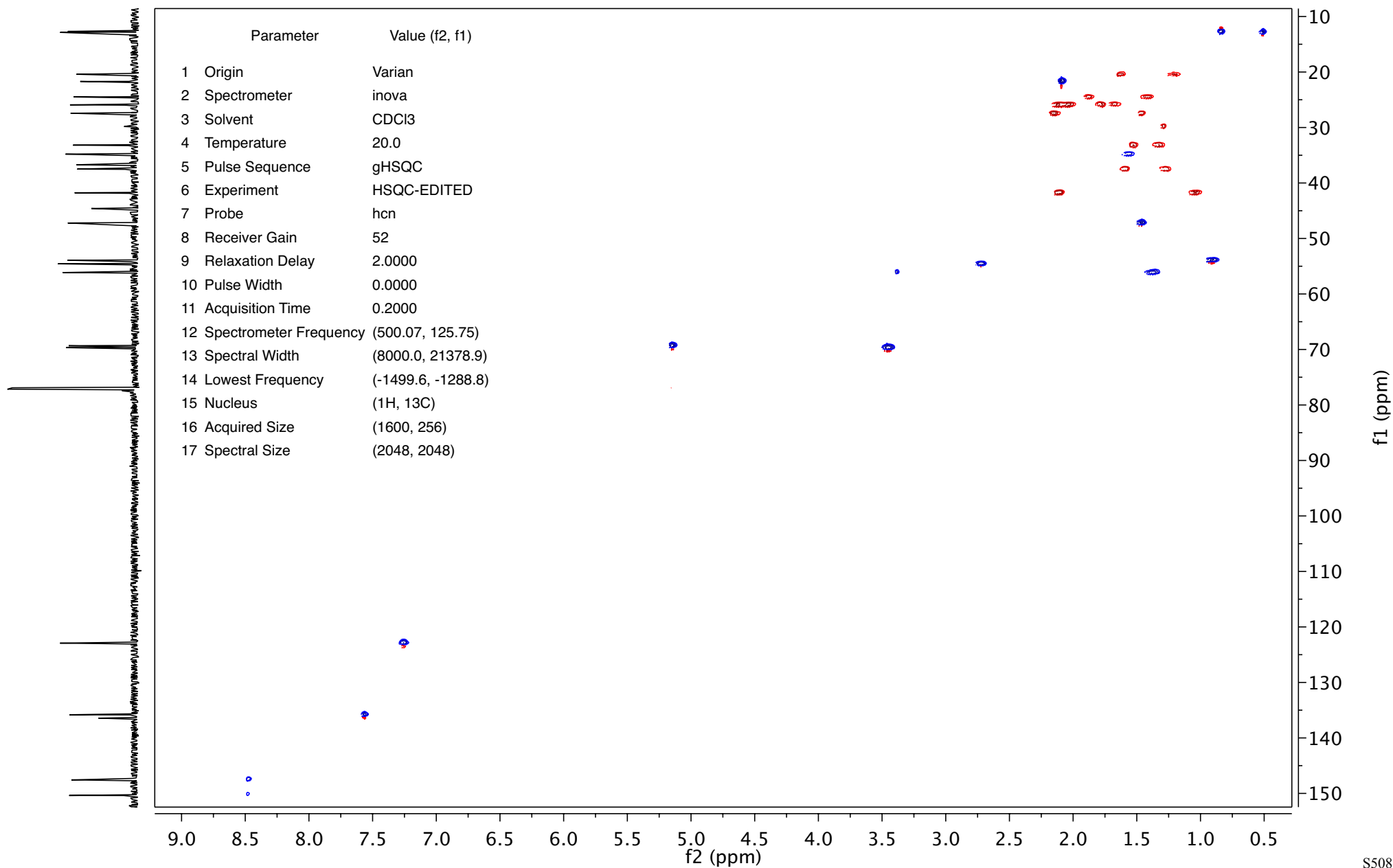
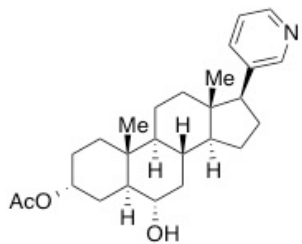


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1274.8
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

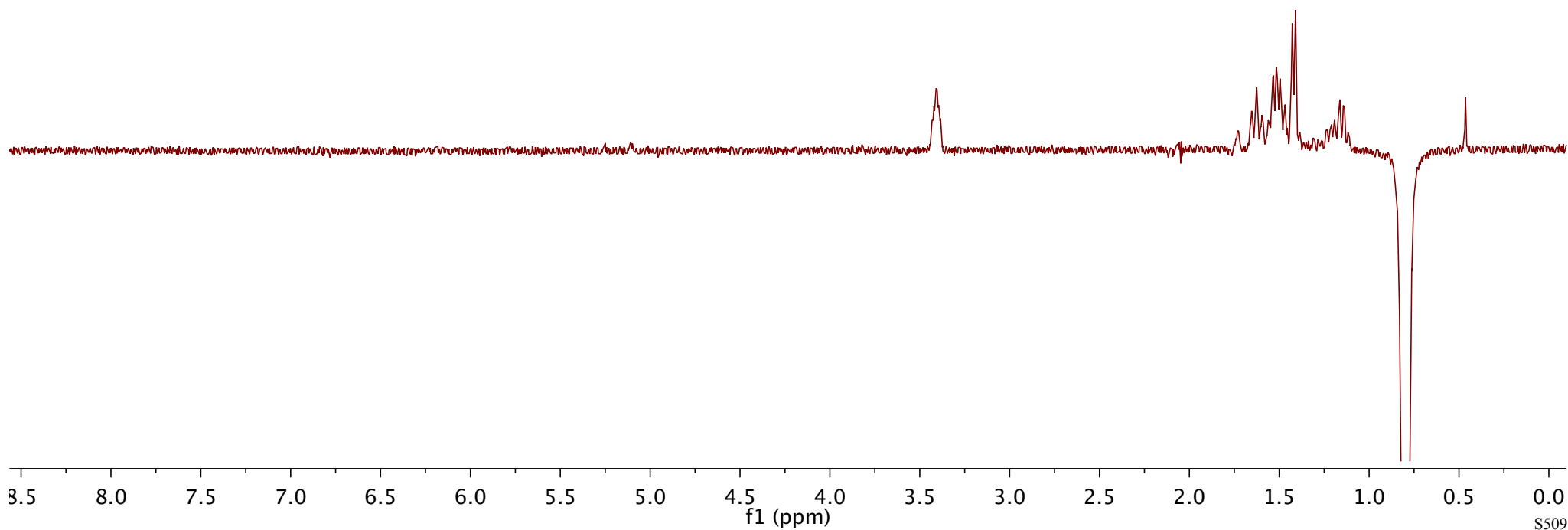
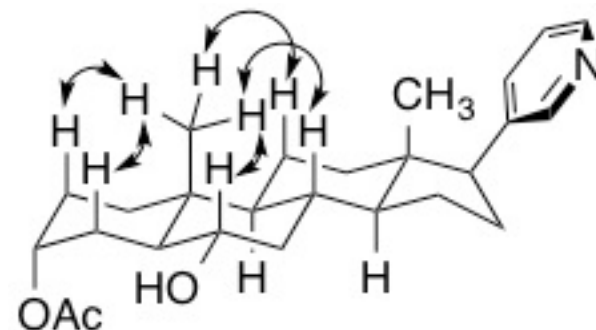




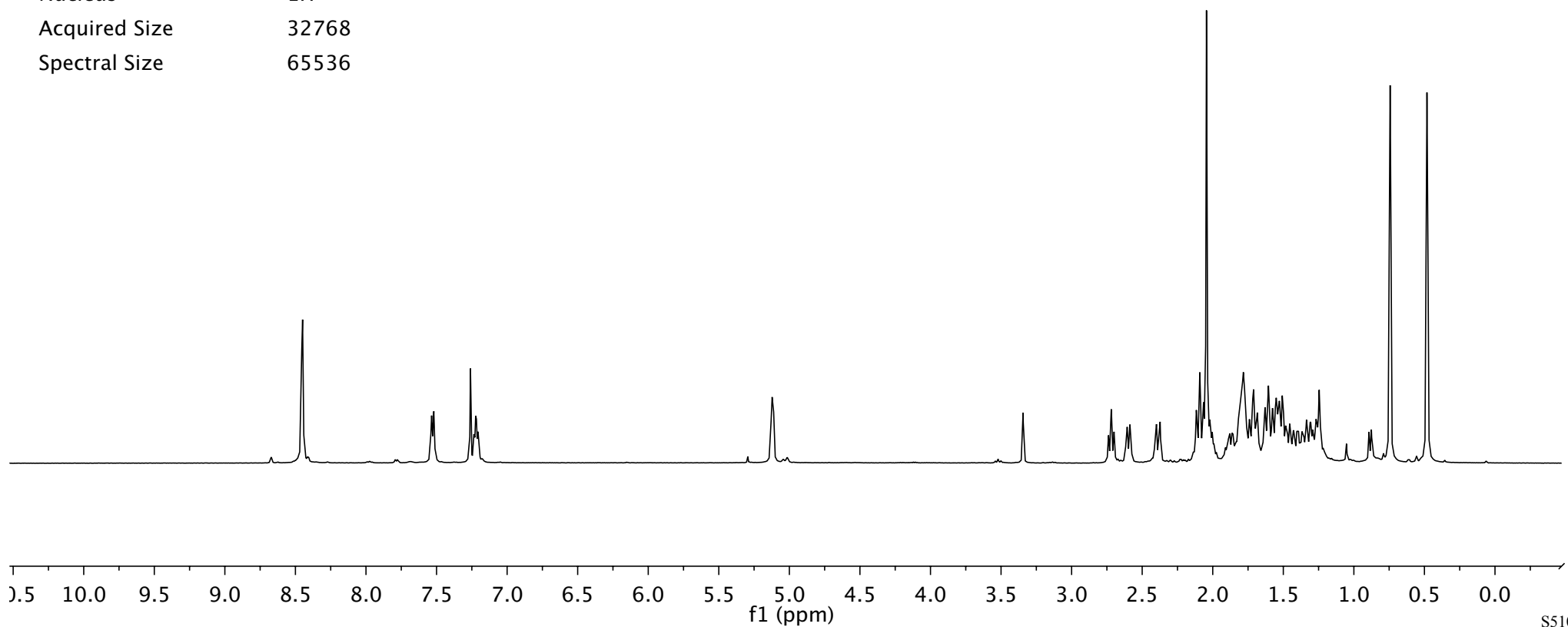
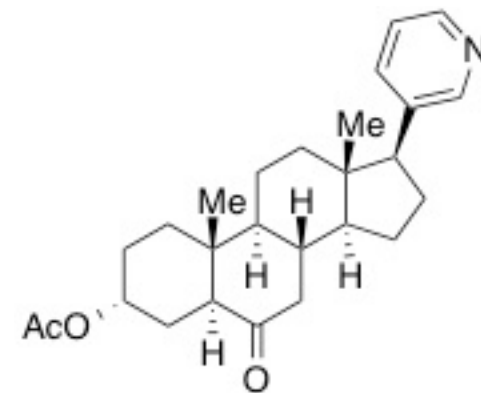


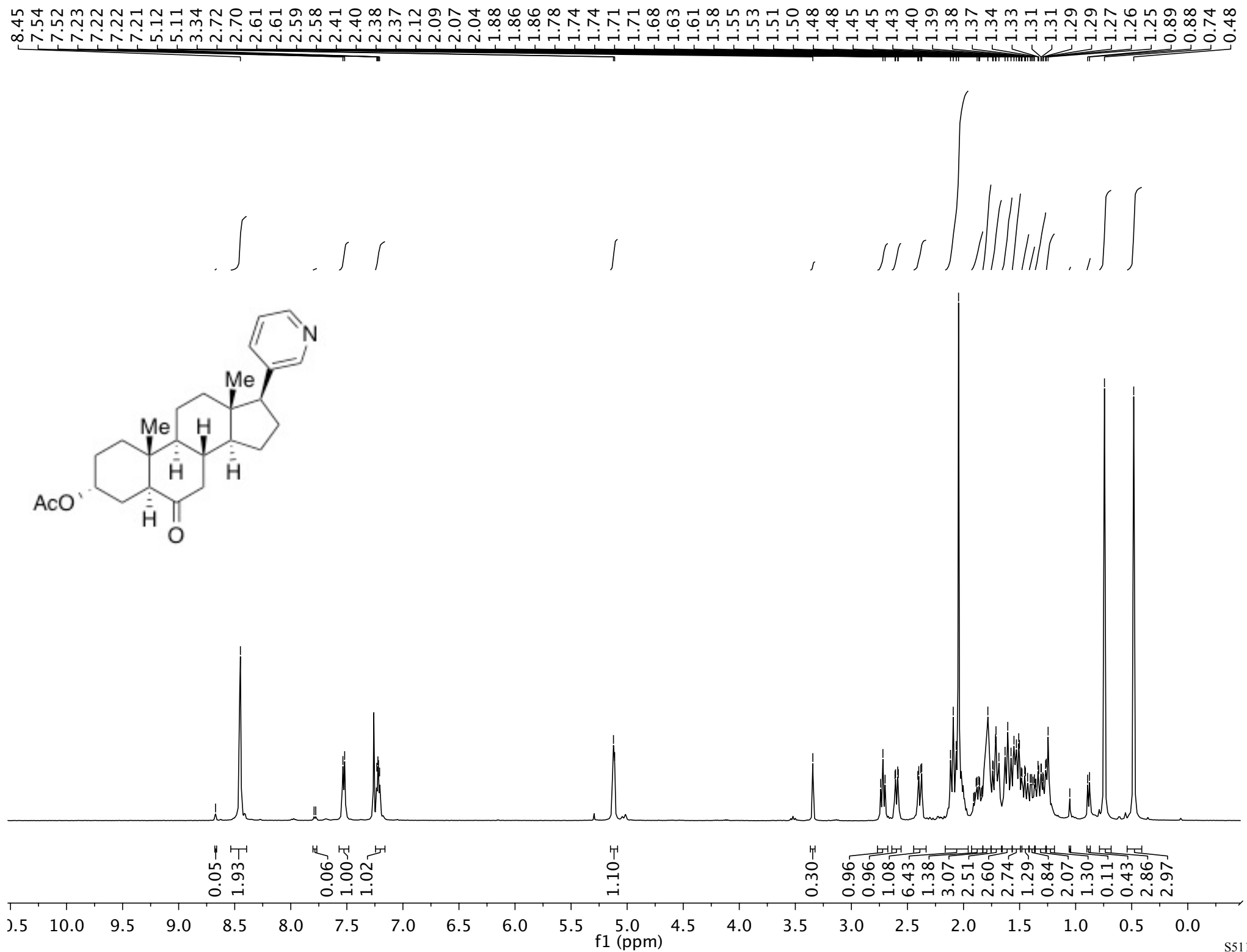


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	NOESY1D
Experiment	1D-NOESY
Probe	hcn
Receiver Gain	44
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1520.9
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

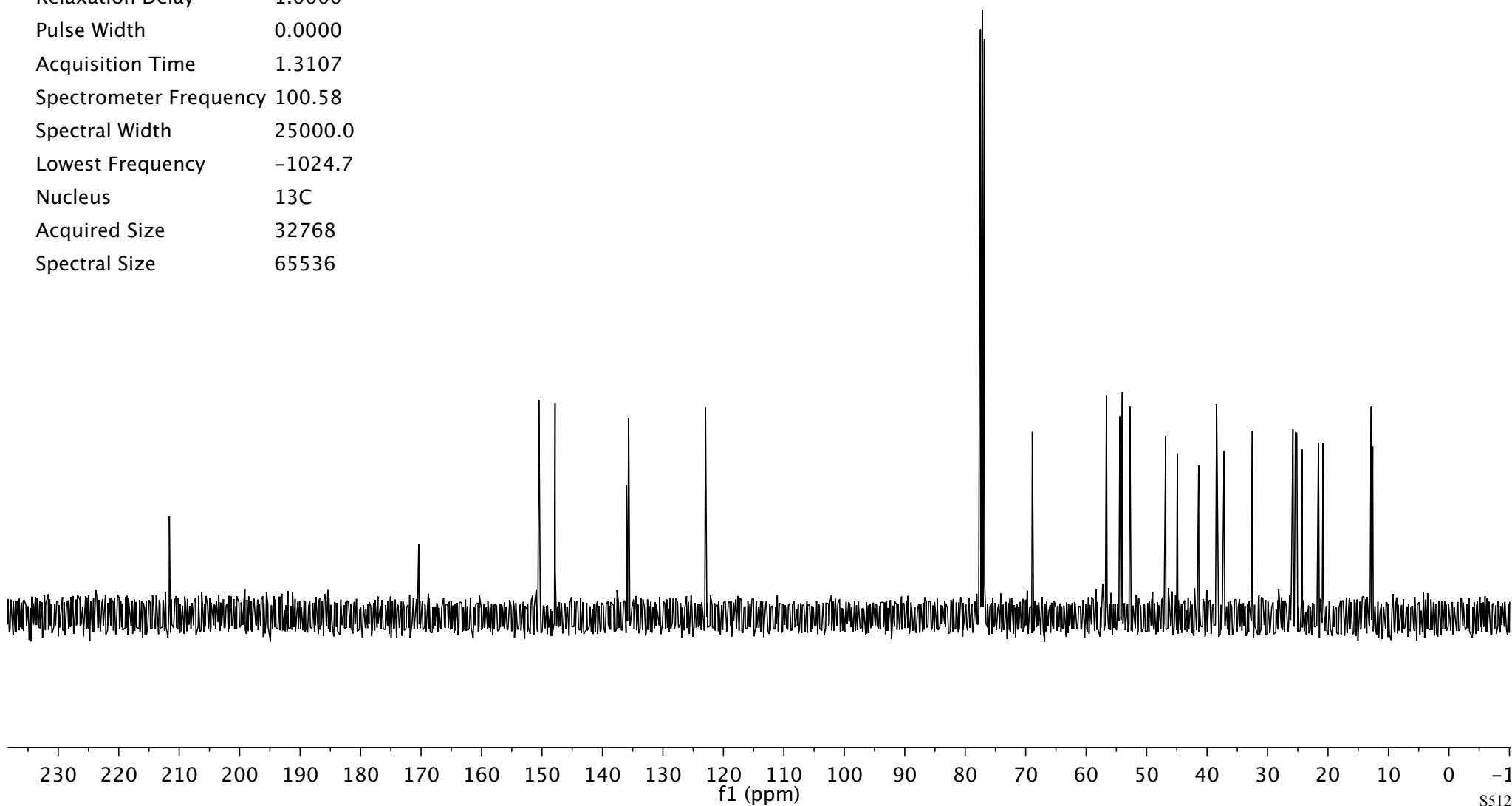
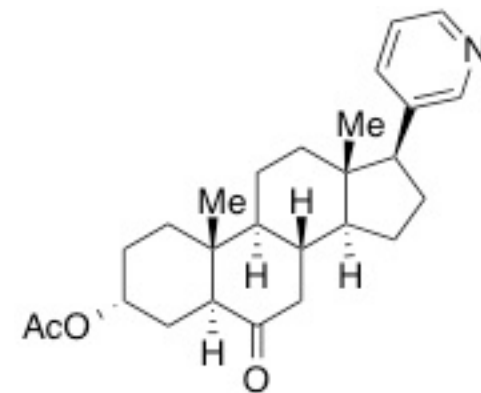


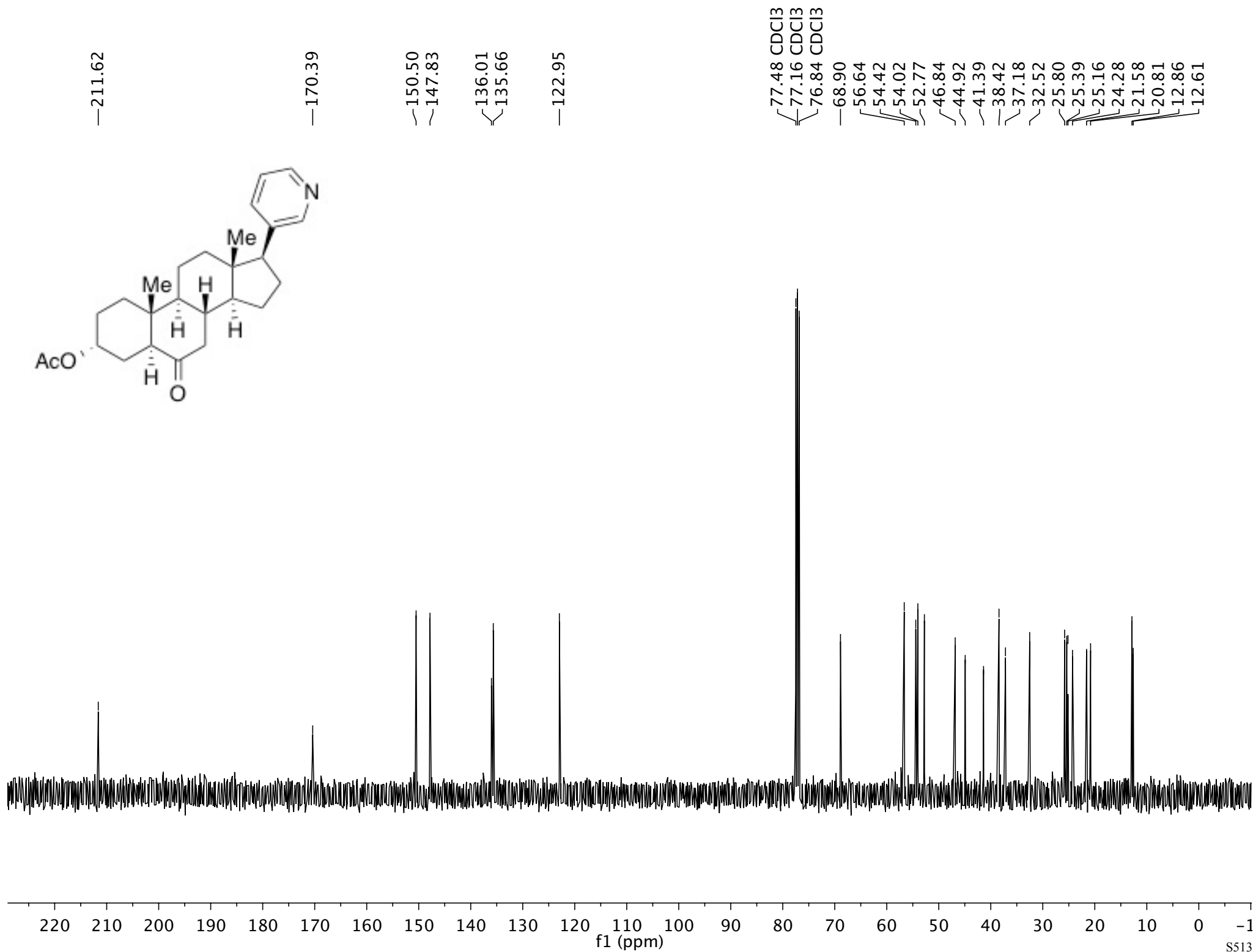
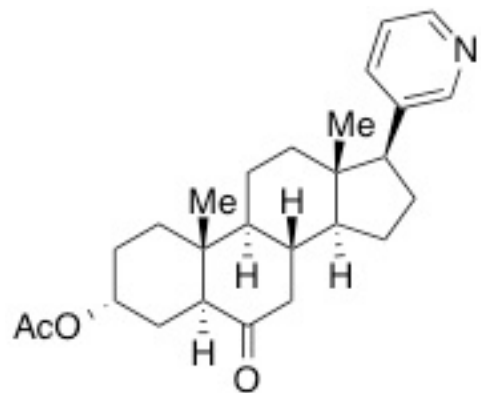
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	44
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1520.4
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

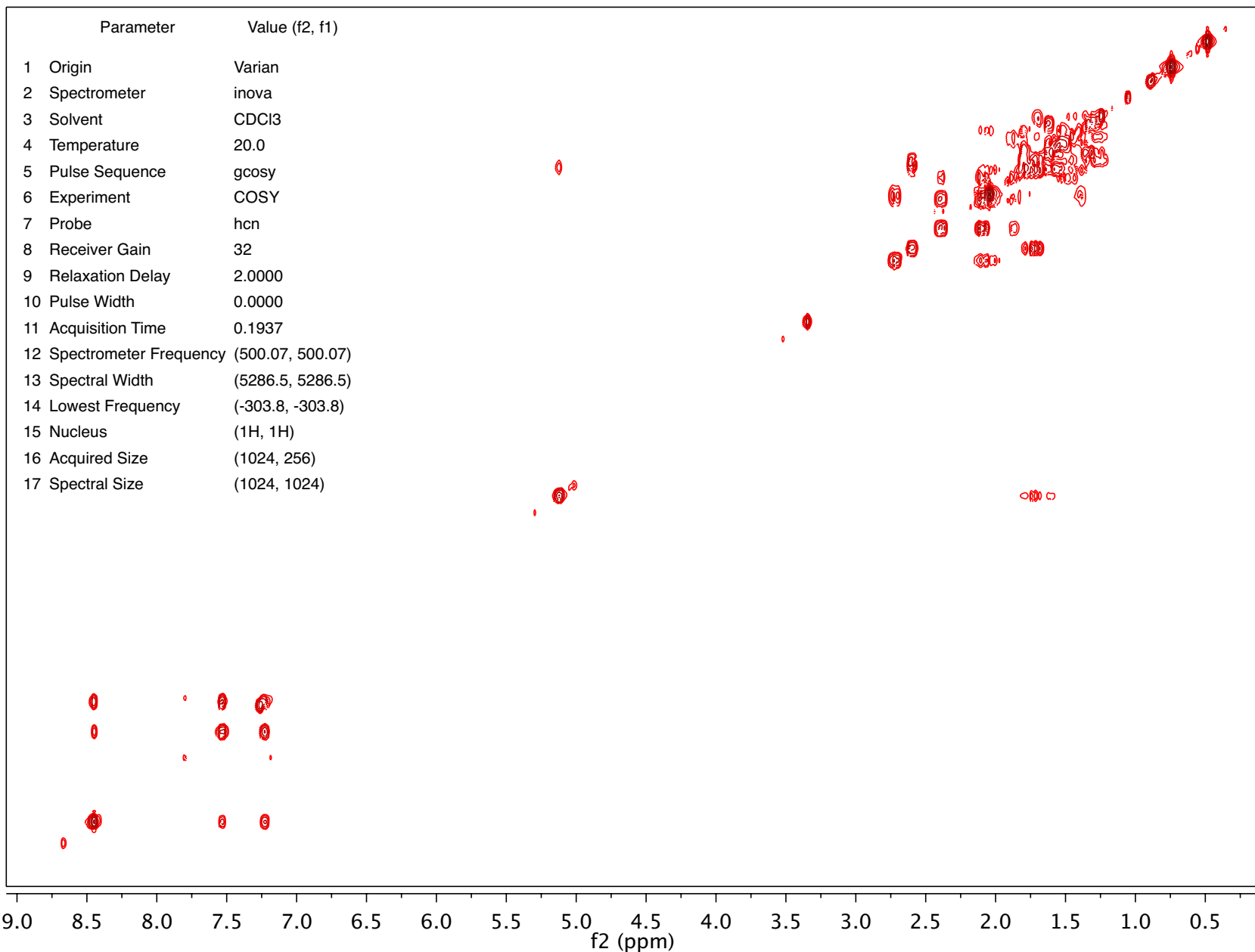
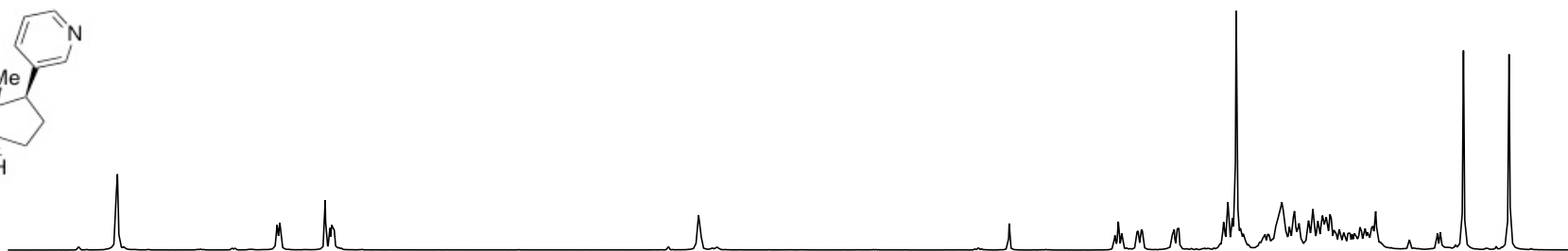
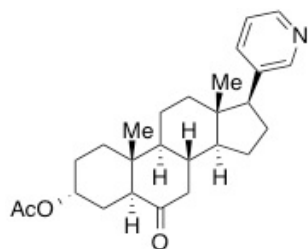


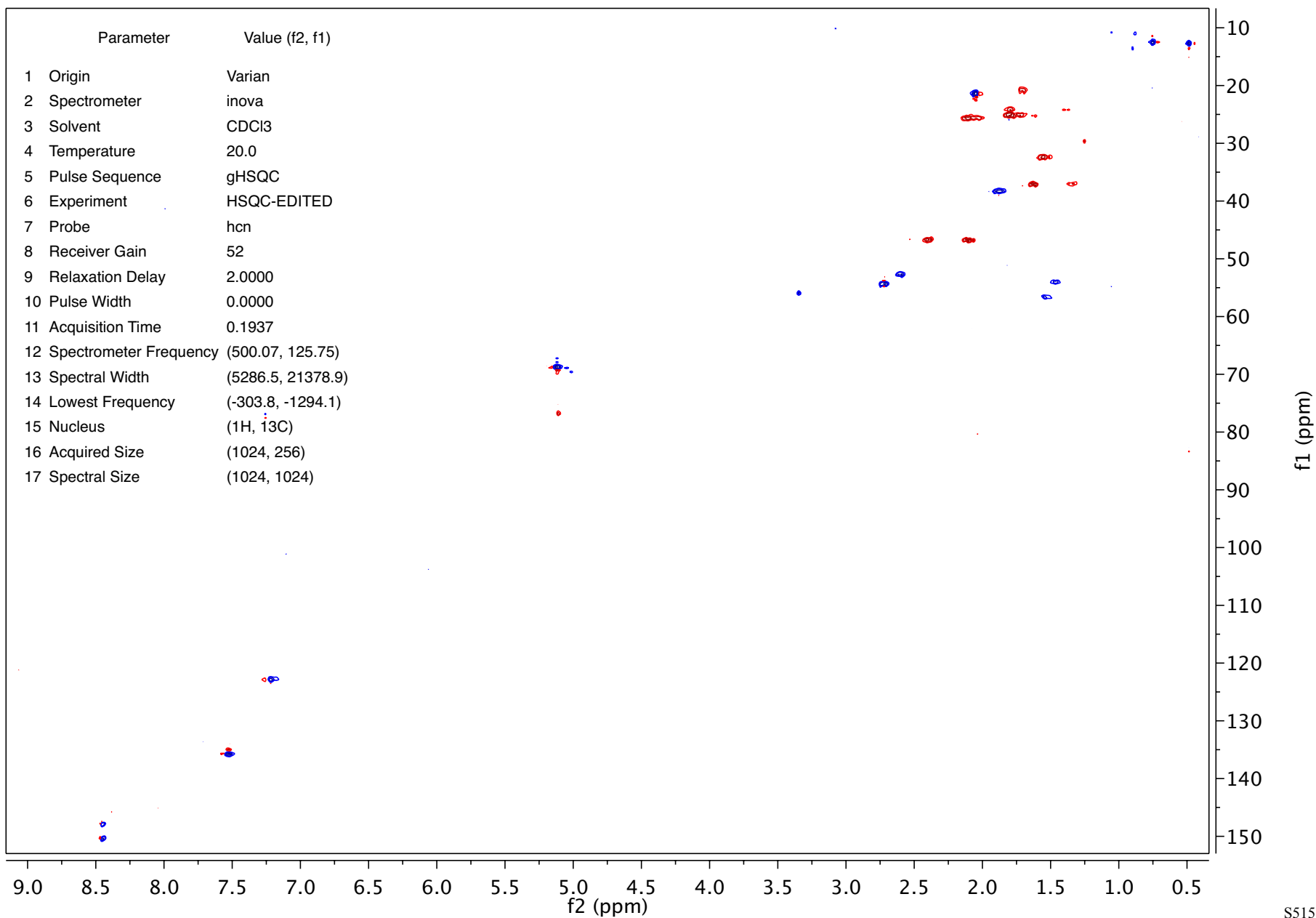
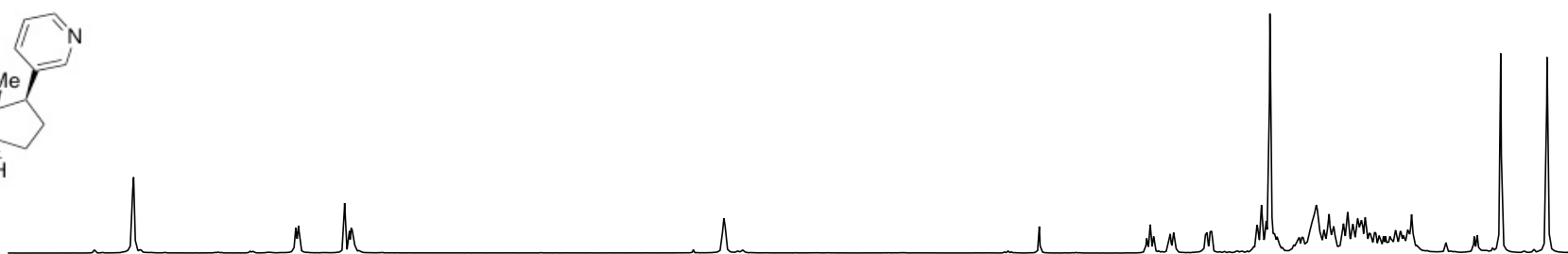
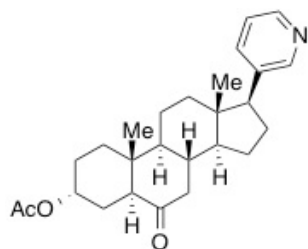


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3107
Spectrometer Frequency	100.58
Spectral Width	25000.0
Lowest Frequency	-1024.7
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



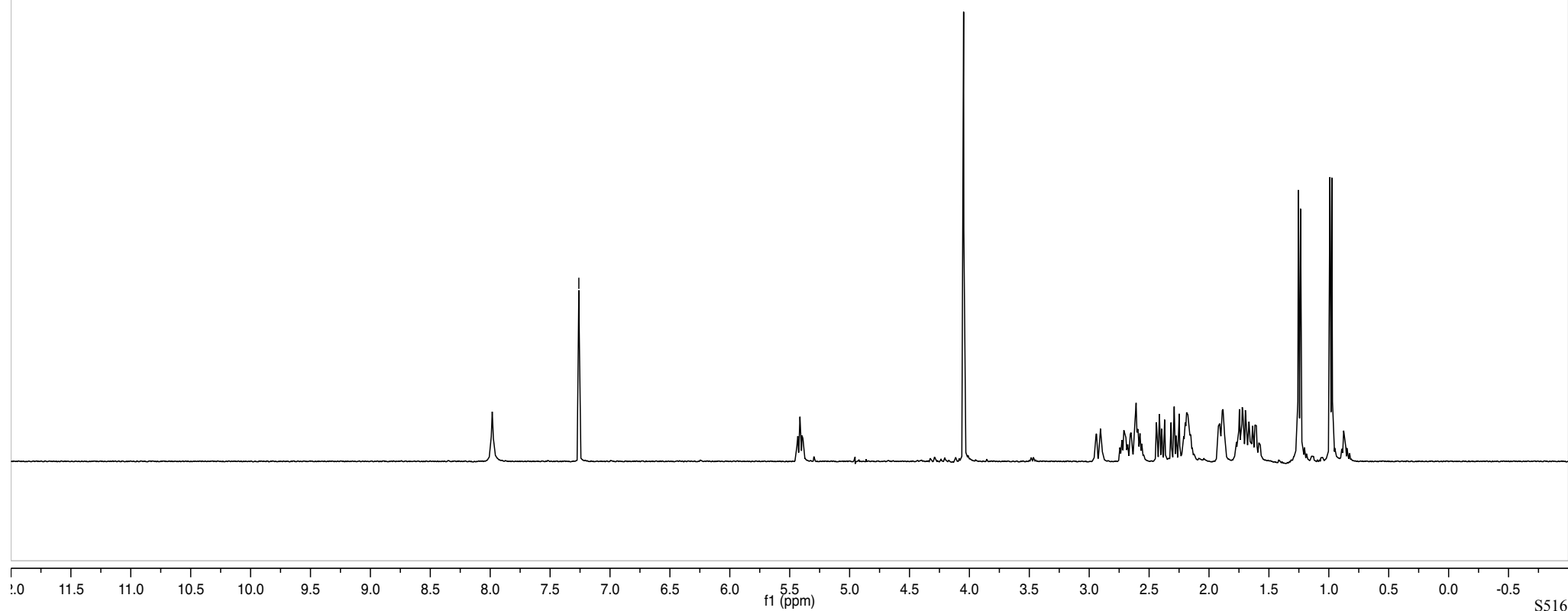
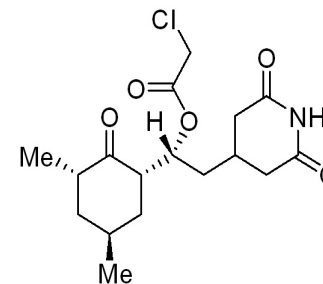


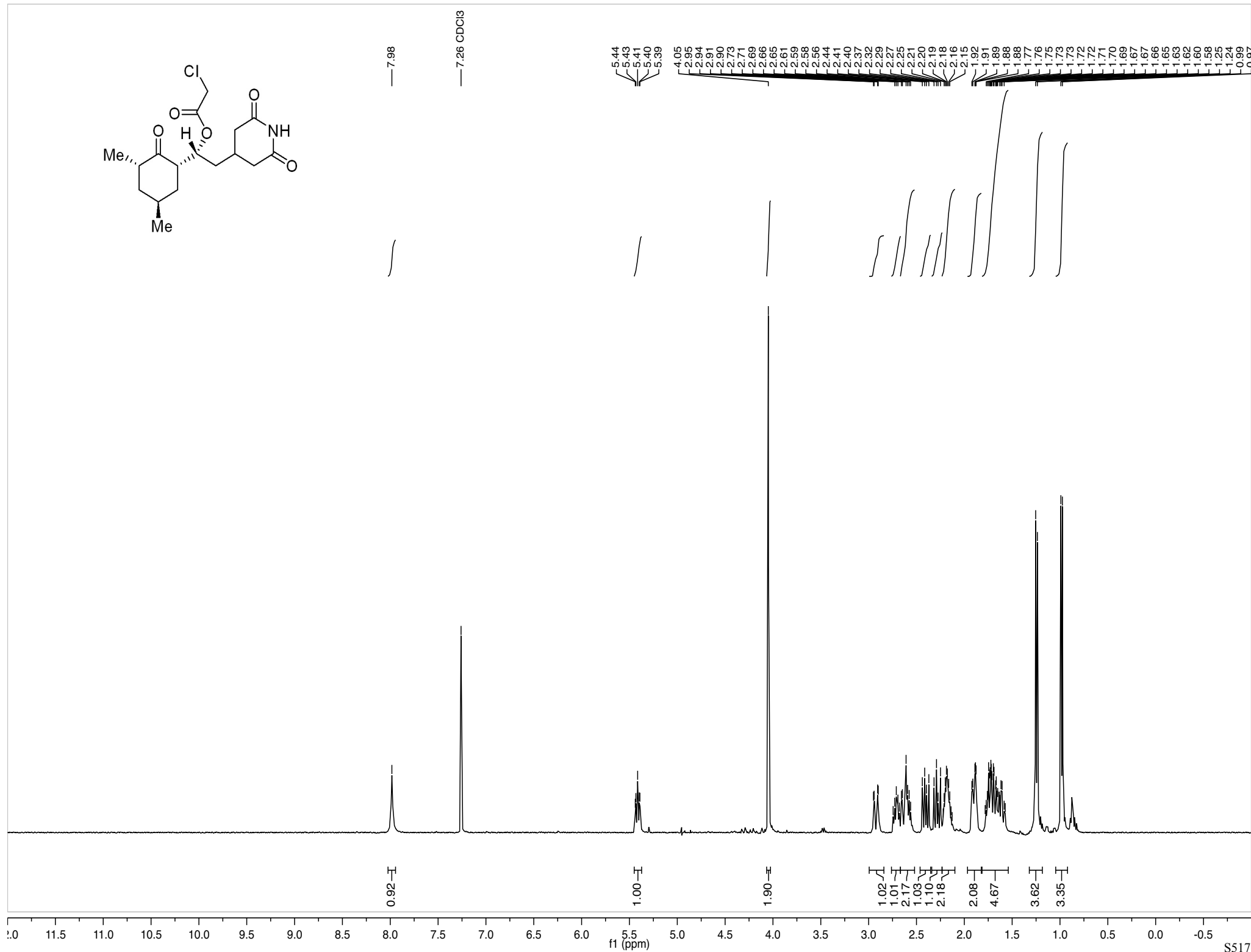
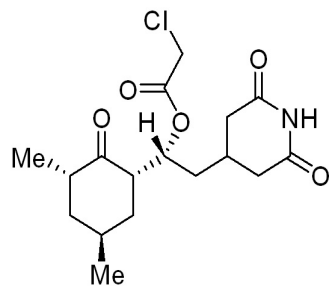




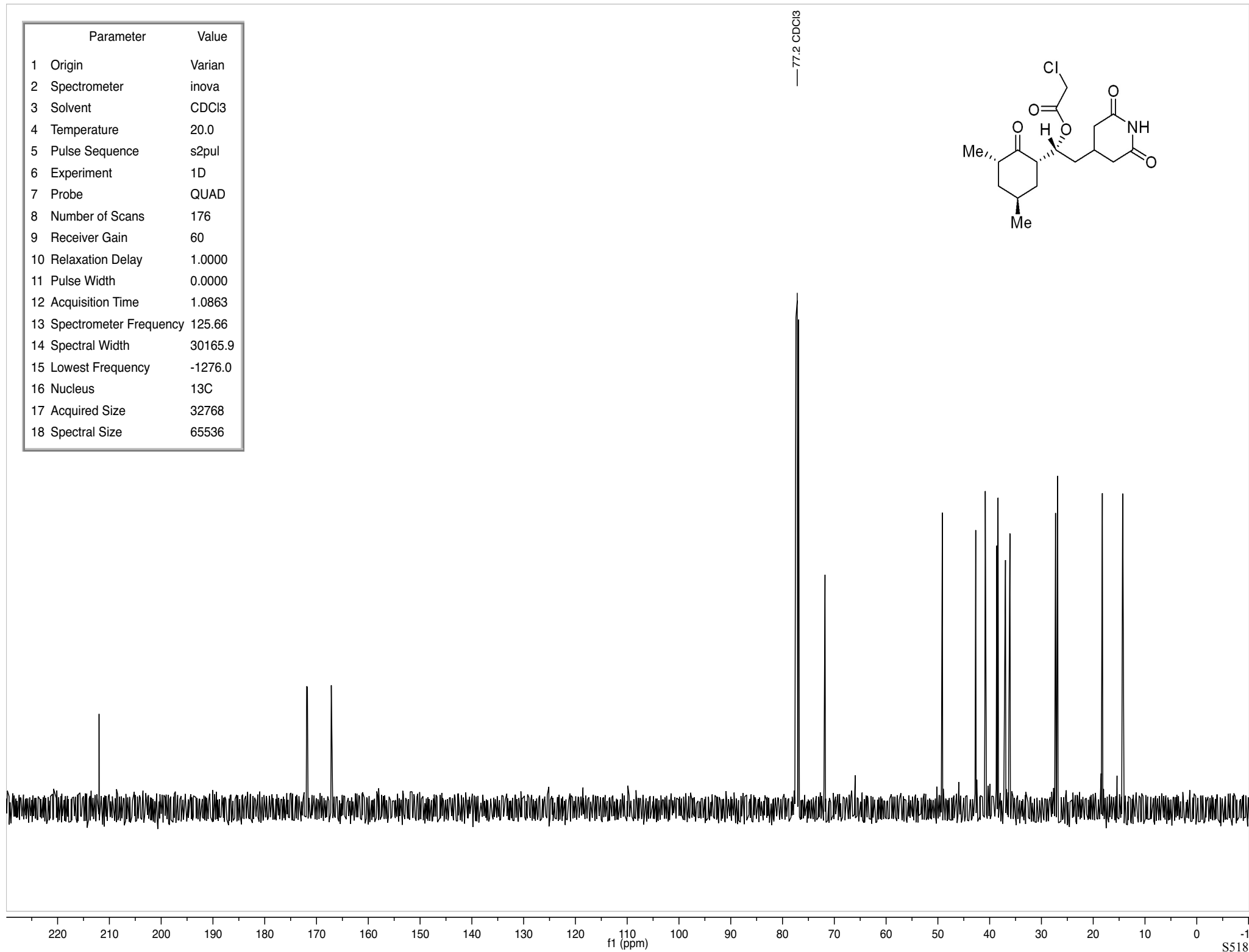
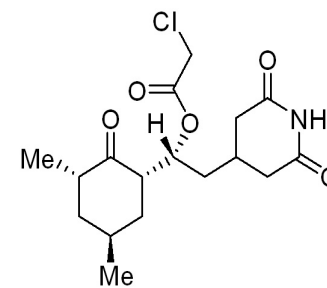
Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl ₃
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	quad94
8 Number of Scans	8
9 Receiver Gain	56
10 Relaxation Delay	0.0000
11 Pulse Width	0.0000
12 Acquisition Time	4.0960
13 Spectrometer Frequency	399.95
14 Spectral Width	8000.0
15 Lowest Frequency	-2424.5
16 Nucleus	¹ H
17 Acquired Size	32768
18 Spectral Size	65536

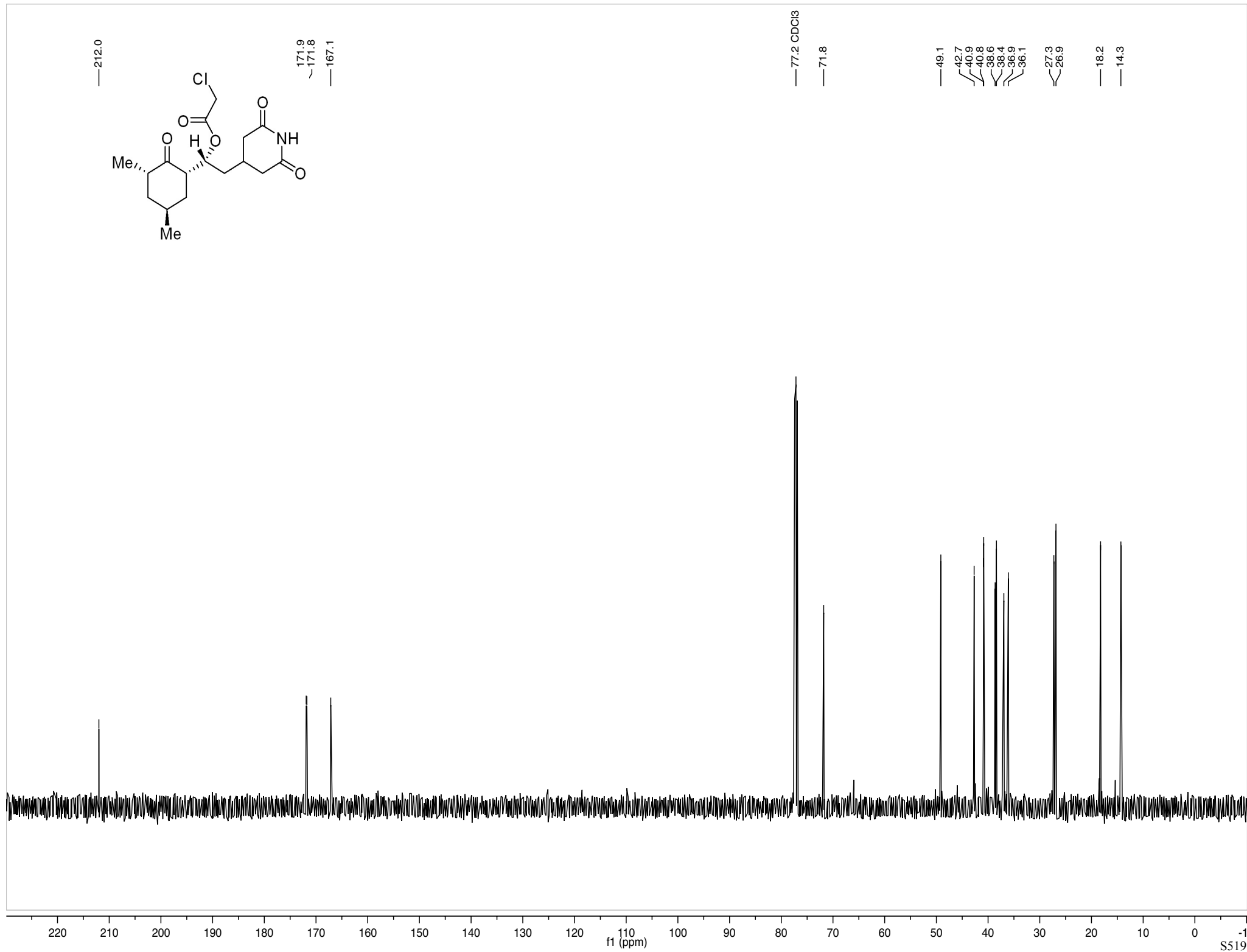
— 7.3 CDCl₃





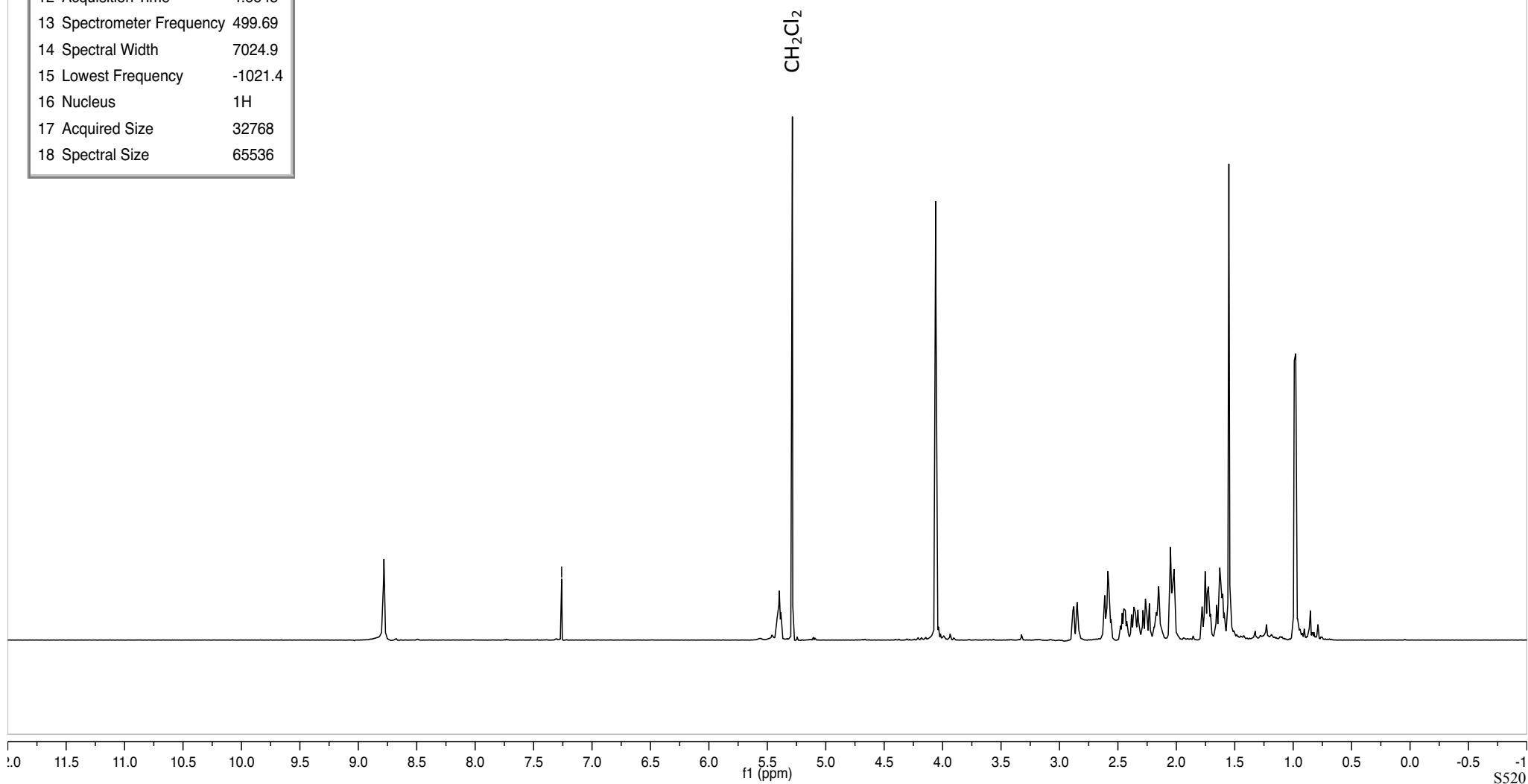
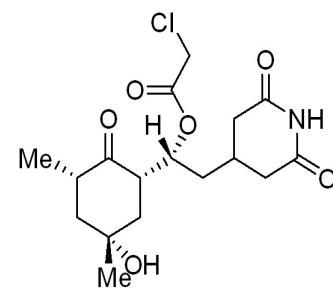
Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	176
9 Receiver Gain	60
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.0863
13 Spectrometer Frequency	125.66
14 Spectral Width	30165.9
15 Lowest Frequency	-1276.0
16 Nucleus	¹³ C
17 Acquired Size	32768
18 Spectral Size	65536

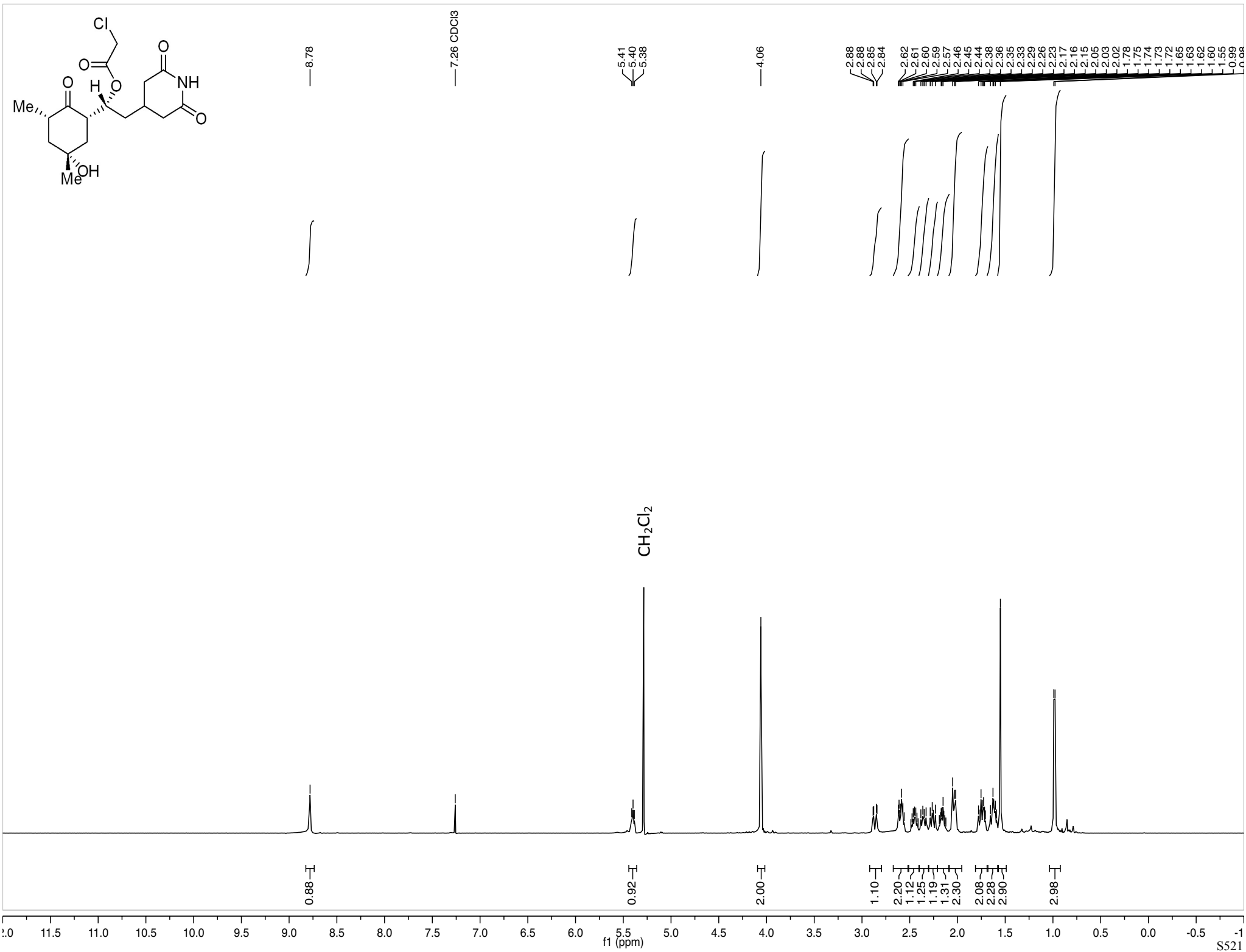




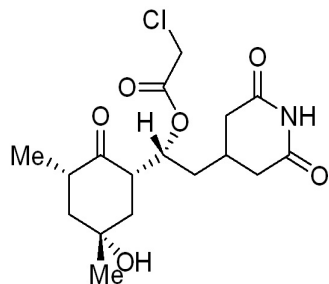
Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl ₃
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	8
9 Receiver Gain	38
10 Relaxation Delay	0.0000
11 Pulse Width	0.0000
12 Acquisition Time	4.6645
13 Spectrometer Frequency	499.69
14 Spectral Width	7024.9
15 Lowest Frequency	-1021.4
16 Nucleus	¹ H
17 Acquired Size	32768
18 Spectral Size	65536

— 7.3 CDCl₃





Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	480
9 Receiver Gain	60
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.0863
13 Spectrometer Frequency	125.66
14 Spectral Width	30165.9
15 Lowest Frequency	-1279.9
16 Nucleus	13C
17 Acquired Size	32768
18 Spectral Size	65536



— 77.2 CDCl3

