

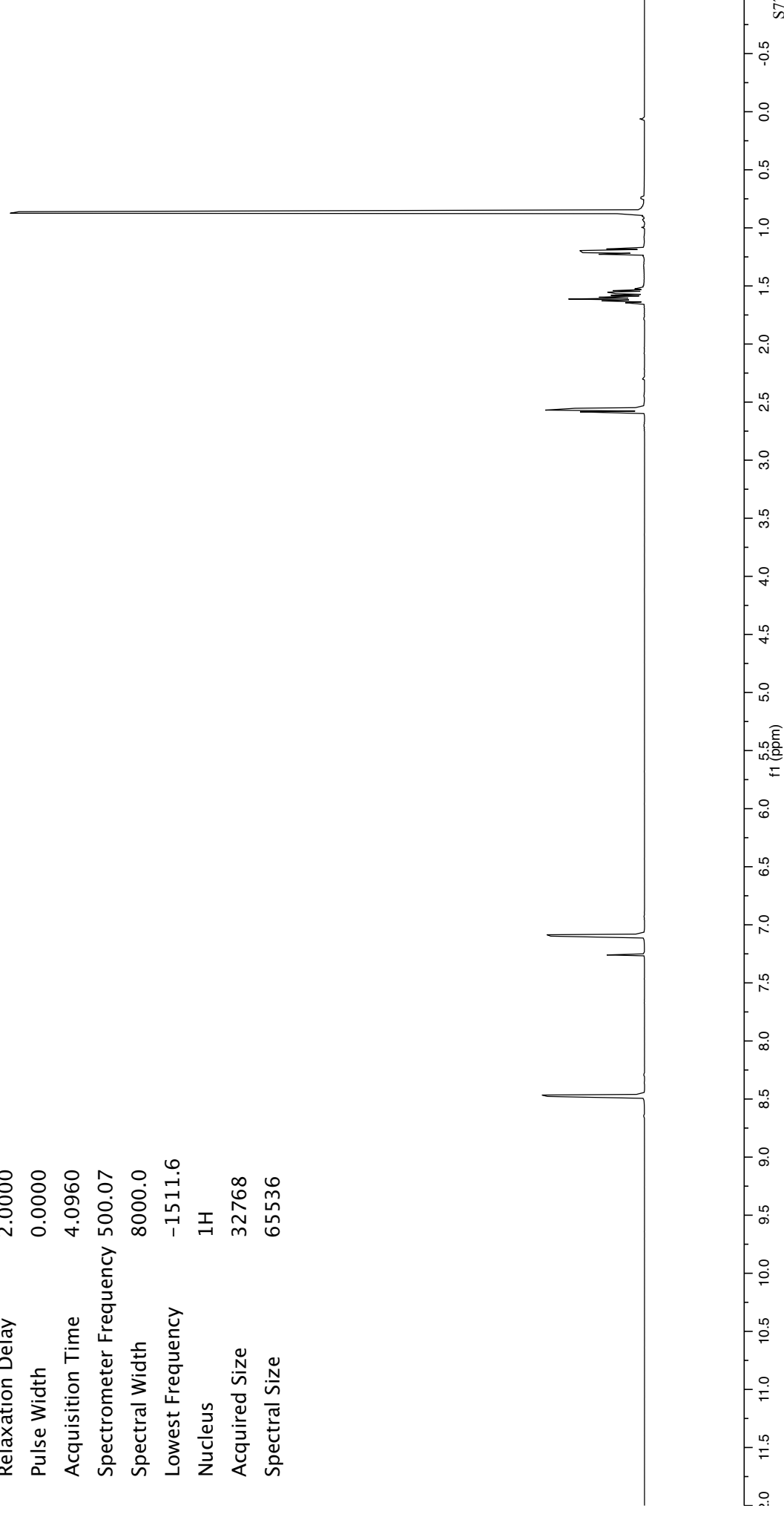
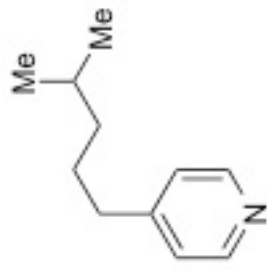
Supporting Information: Spectra Data

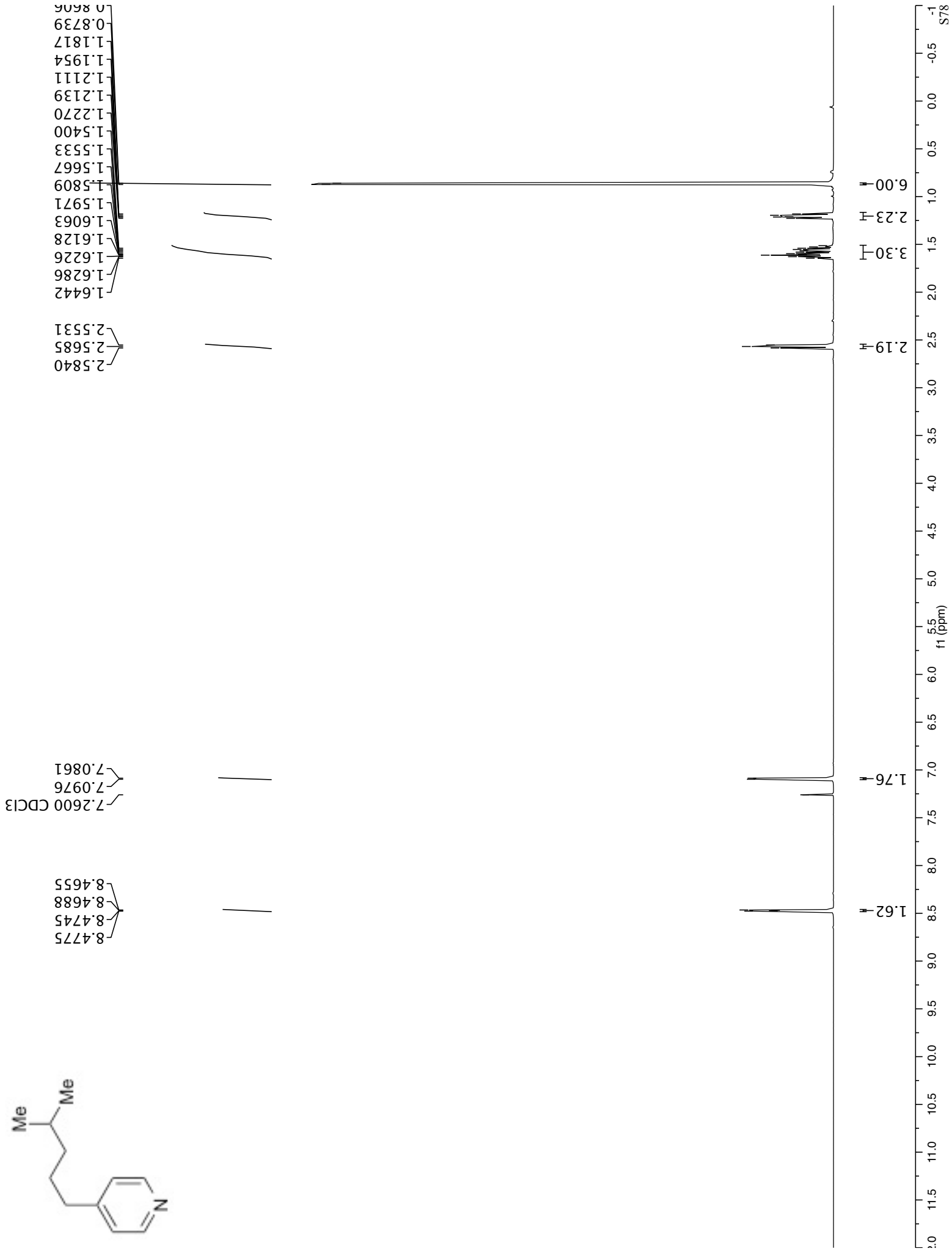
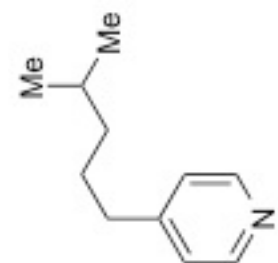
Remote Oxidation of Aliphatic C—H Bonds in Nitrogen-Containing Molecules

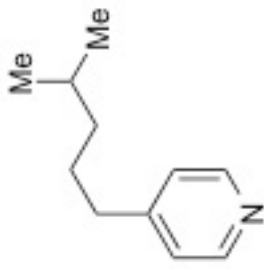
Jennifer M. Howell[‡], Kaibo Feng[‡], Joseph R. Clark, Louis J. Trzepkowski and M. Christina White*

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

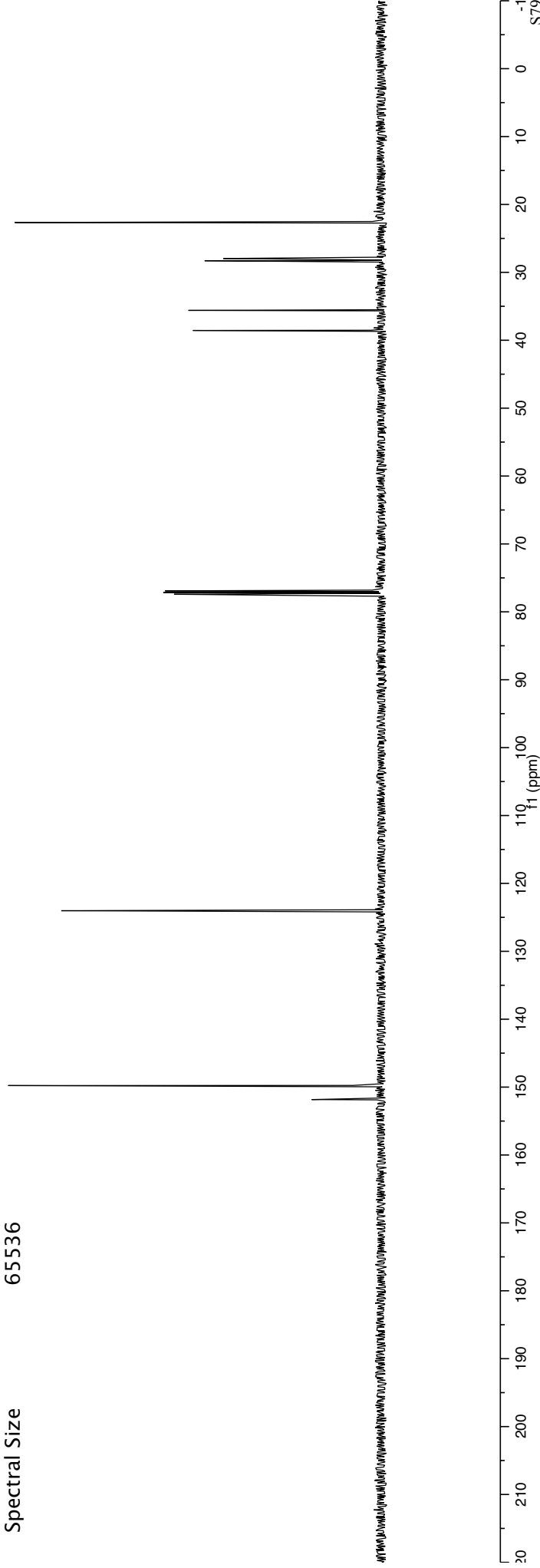
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCI3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	28
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1511.6
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

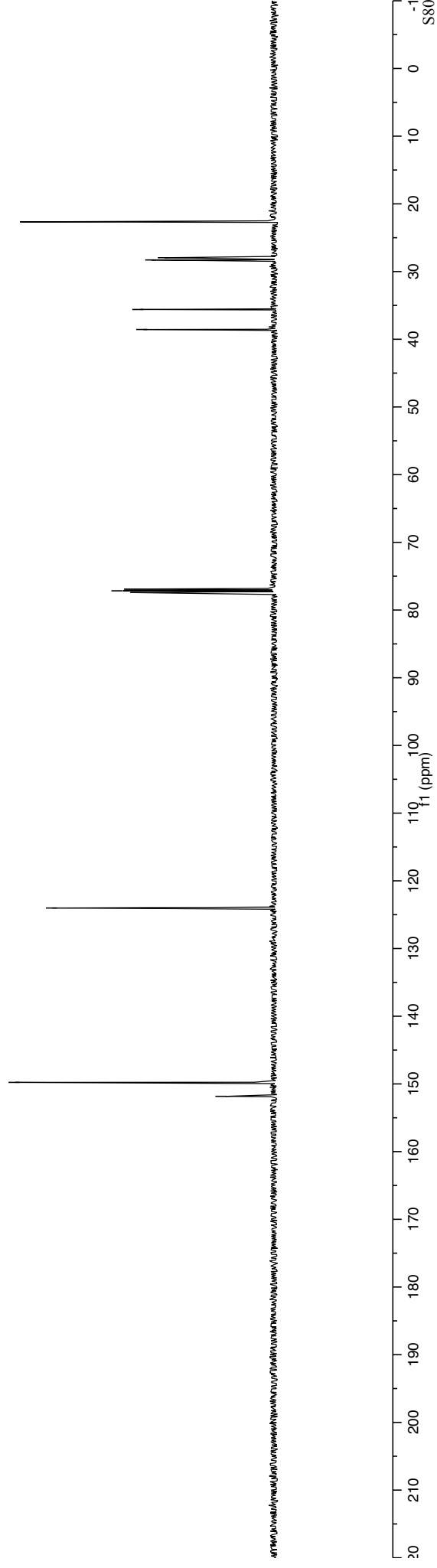
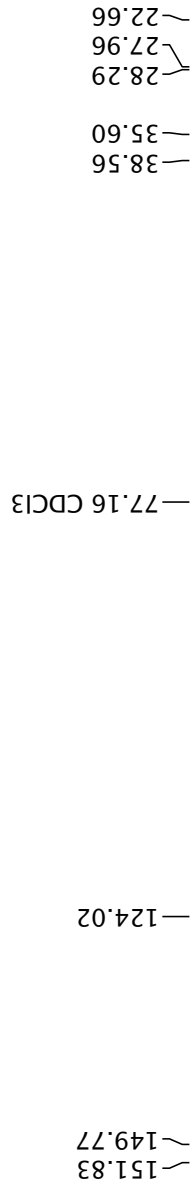
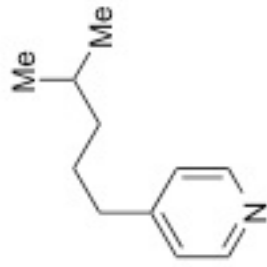


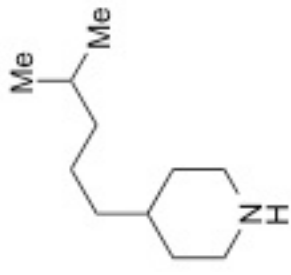




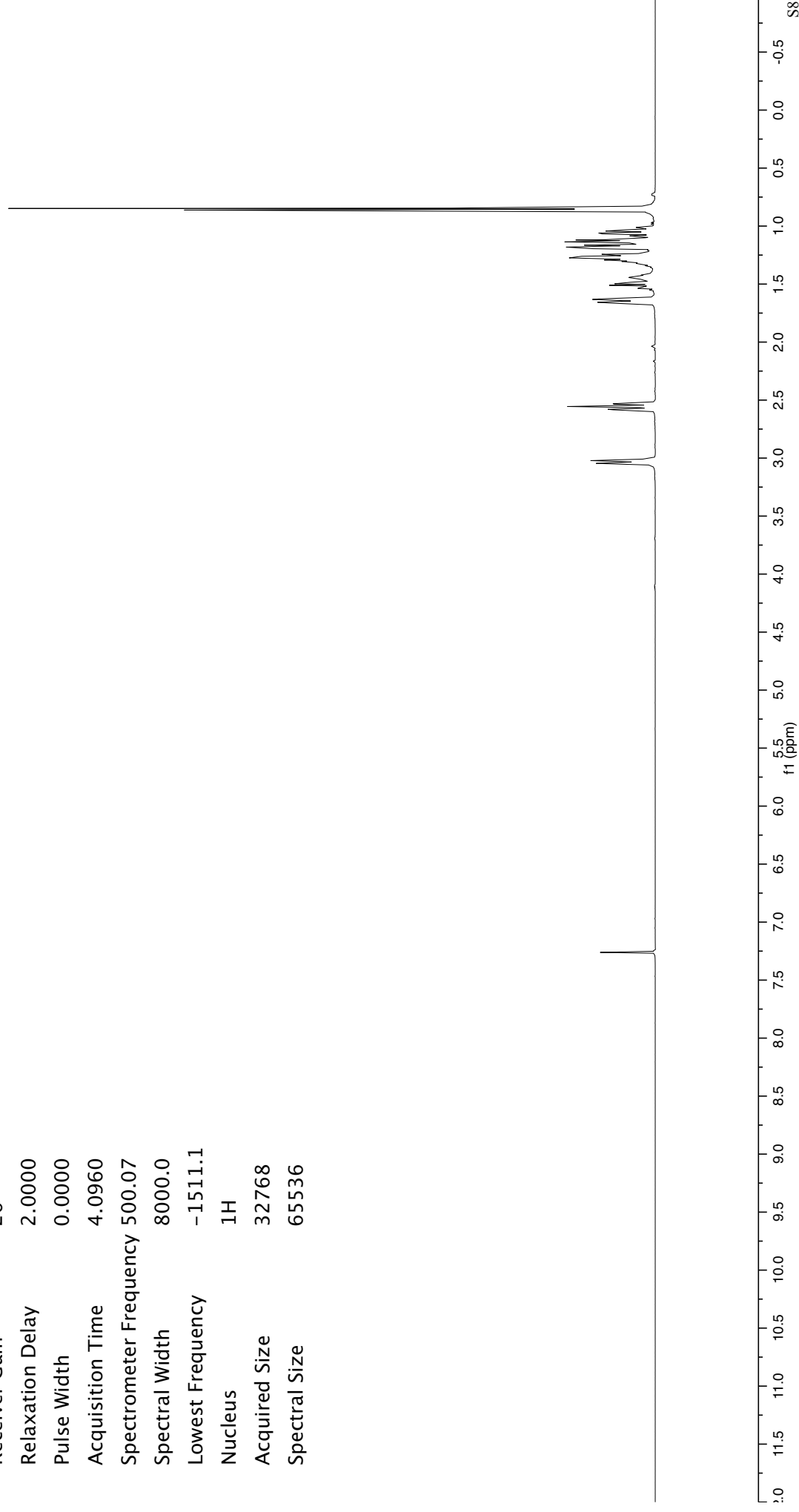
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Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	176
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral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

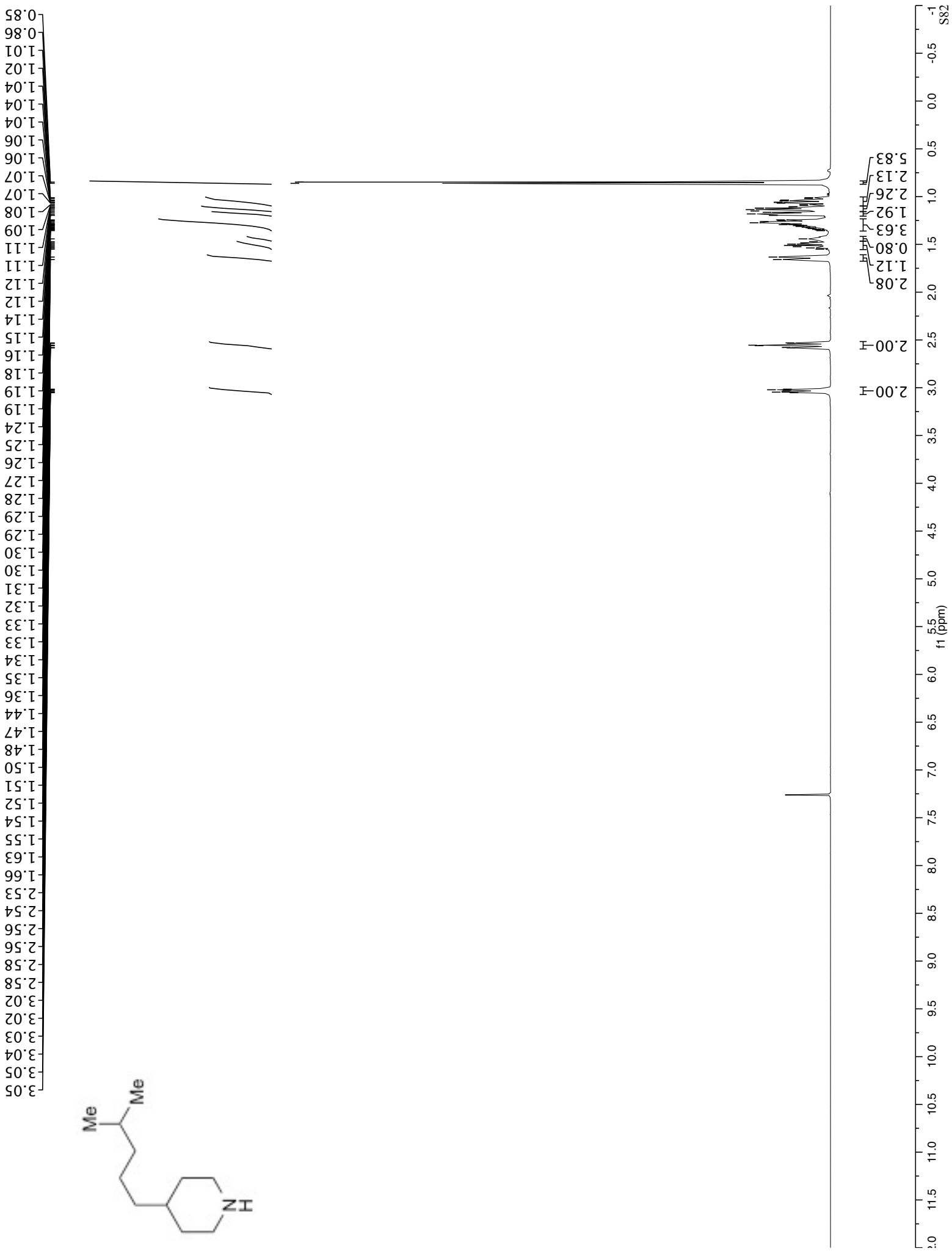
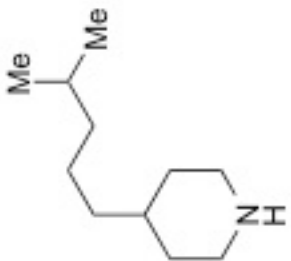


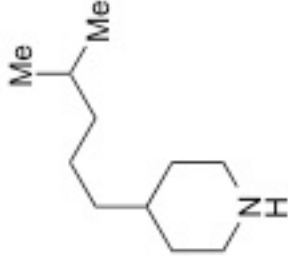




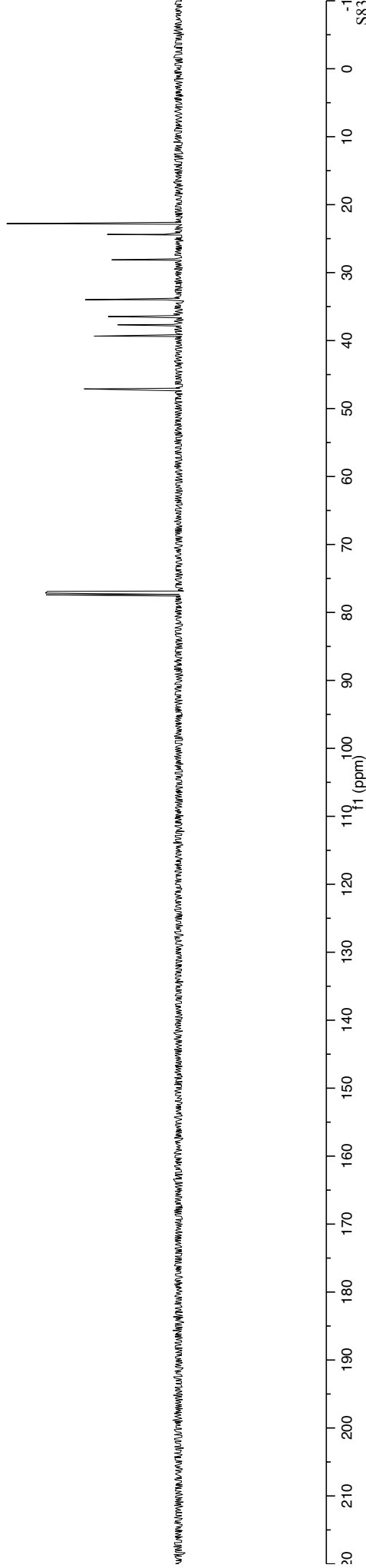
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Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	26
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-15111.1
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

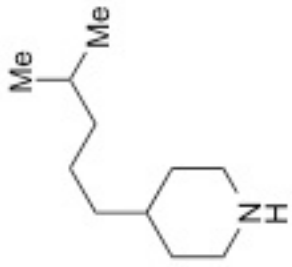






Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	96
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1271.1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





— 77.16 CDCl₃

— 47.11

— 39.34

— 37.68

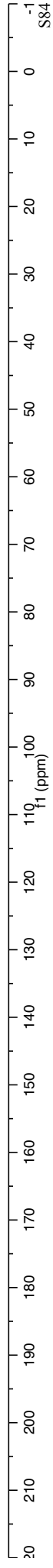
— 36.47

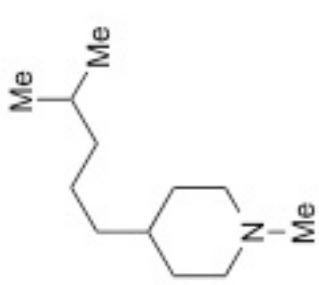
— 33.98

— 28.11

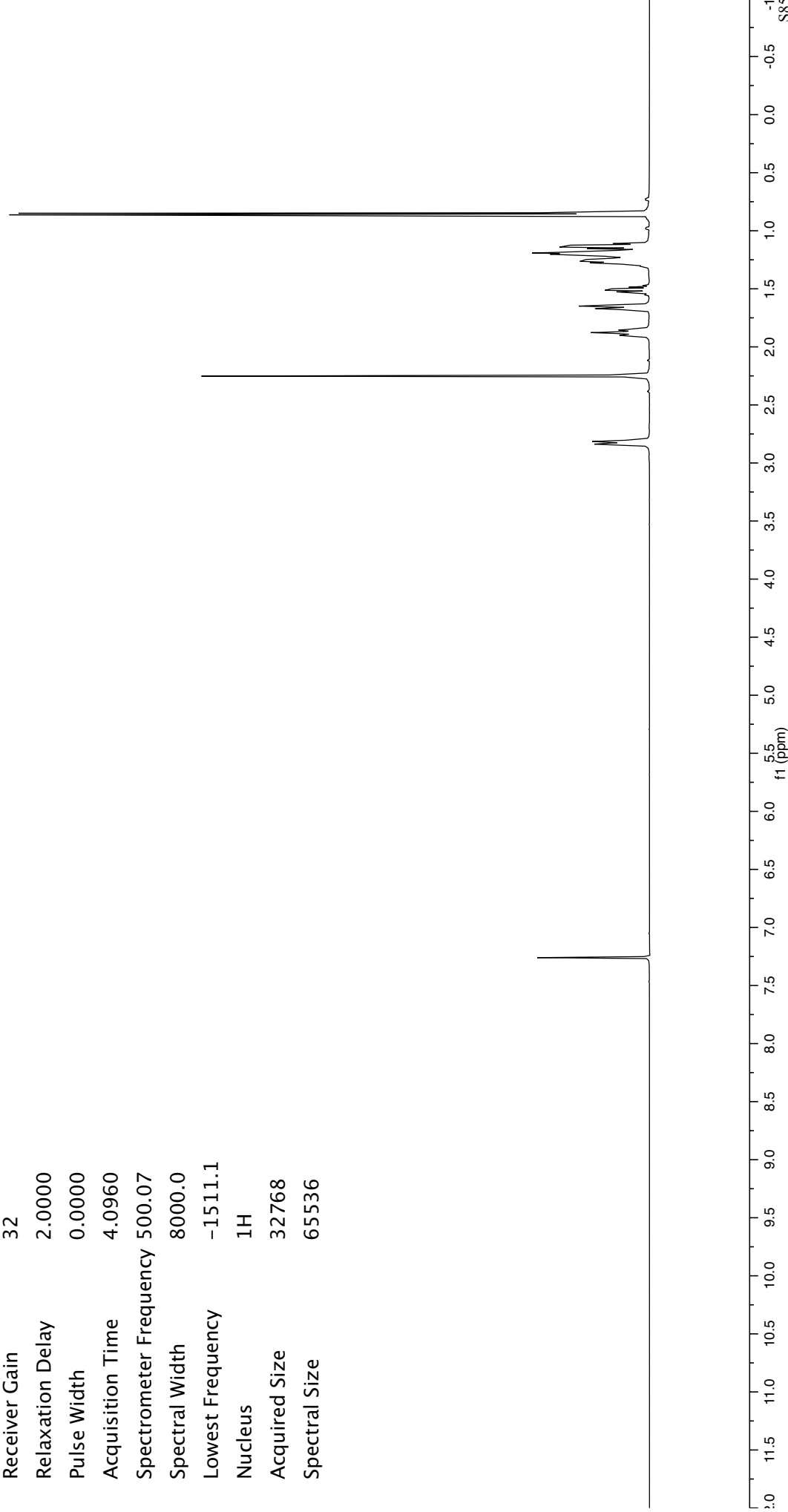
— 24.38

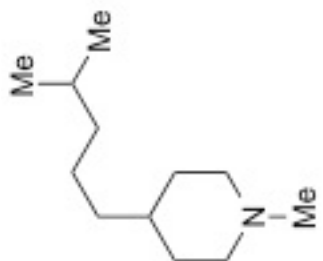
— 22.78



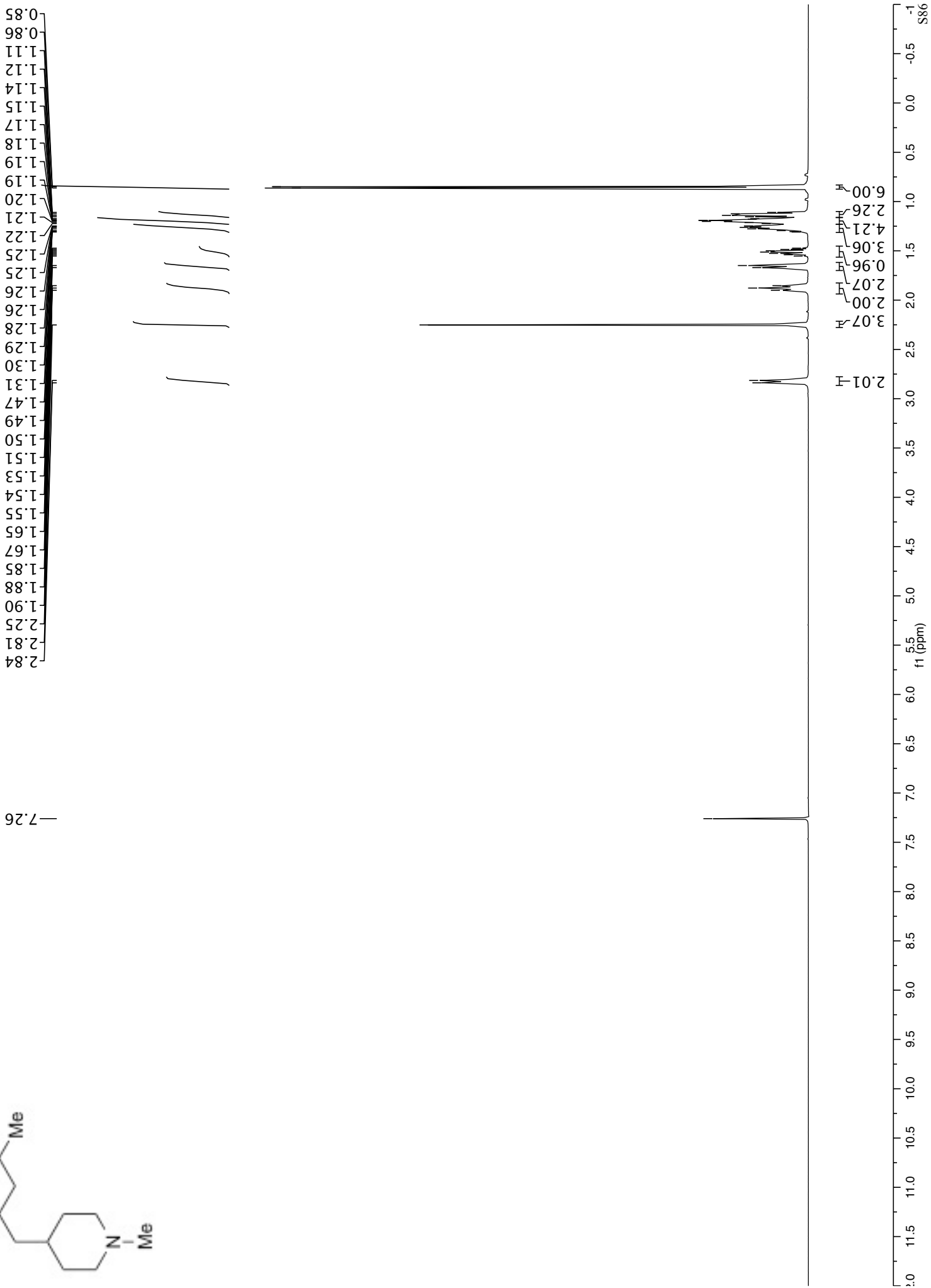


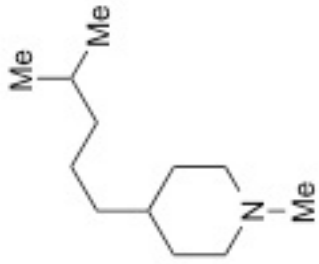
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Title	JMH-III-32_1H
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	32
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-15111.1
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



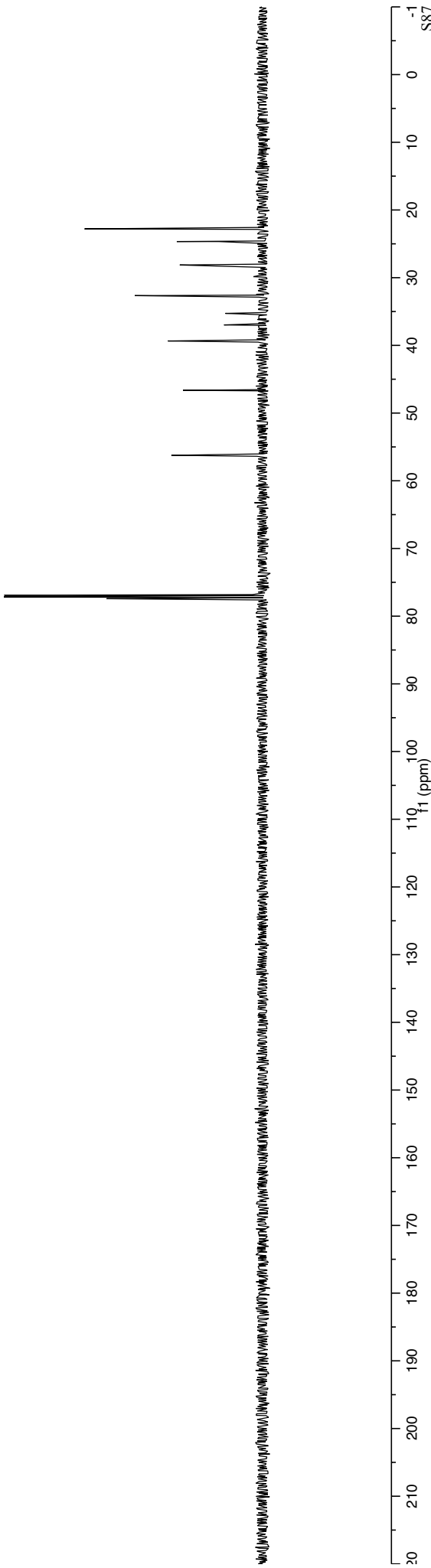


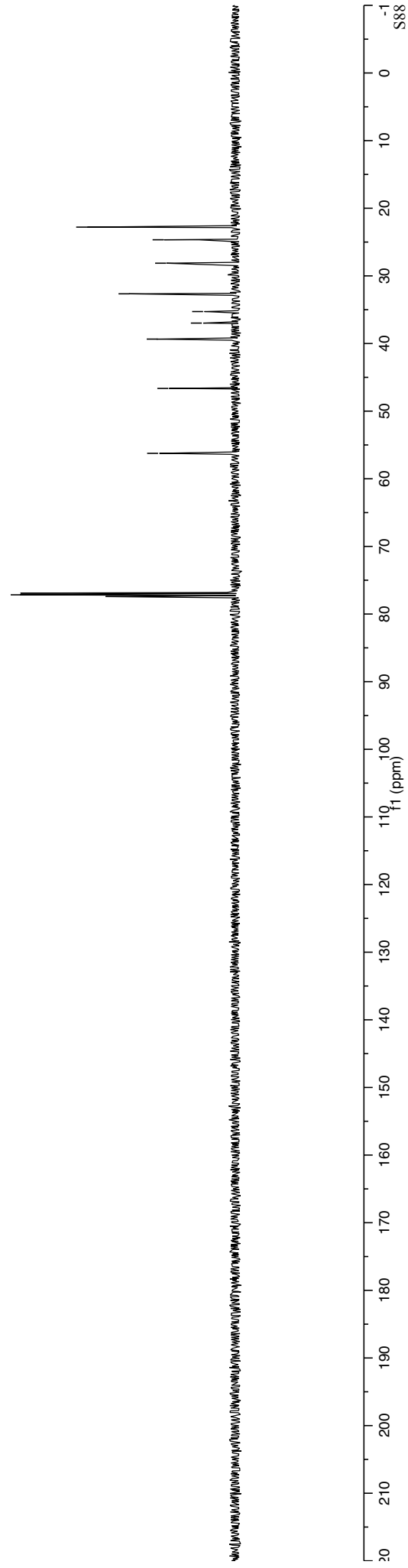
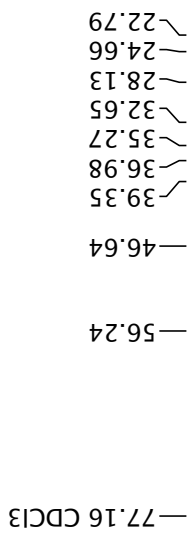
—7.26 CDCl₃

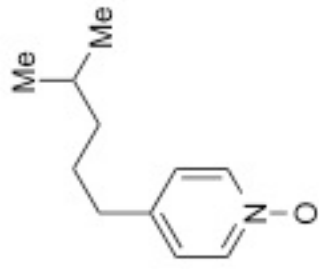




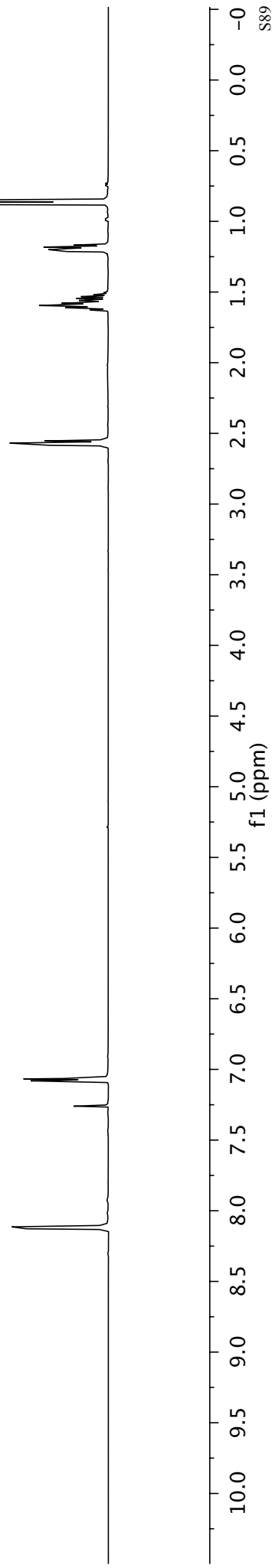
Parameter	Value
Title	JMH-III-22_13C
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	192
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9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

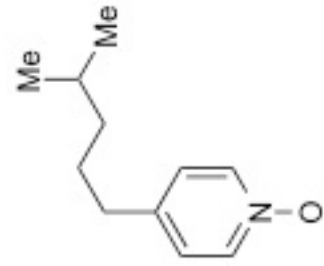






Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	32
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.6
Nucleus	¹ H
Acquired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





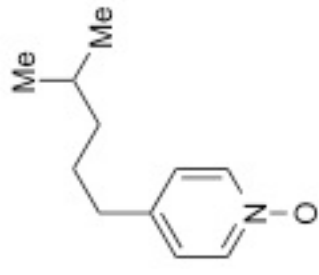
8.13
8.11
7.26 CDCl₃
7.08
7.07

2.58
2.57
2.55
1.63
1.61
1.60
1.58
1.57
1.56
1.56
1.55
1.53
1.21
1.20
1.19
1.18
1.17
0.87
0.86

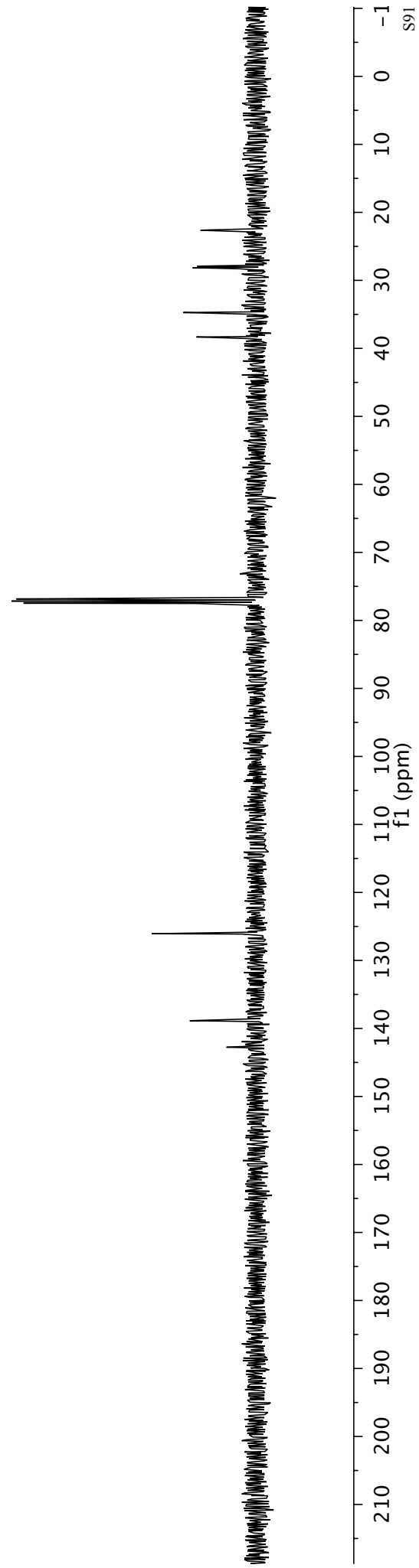
1.68
1.71
2.12
3.00
2.08
6.16

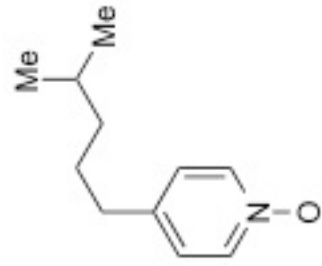
f1 (ppm)

S90



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

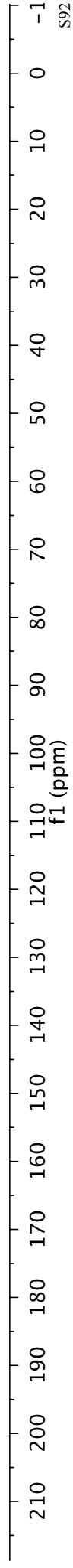


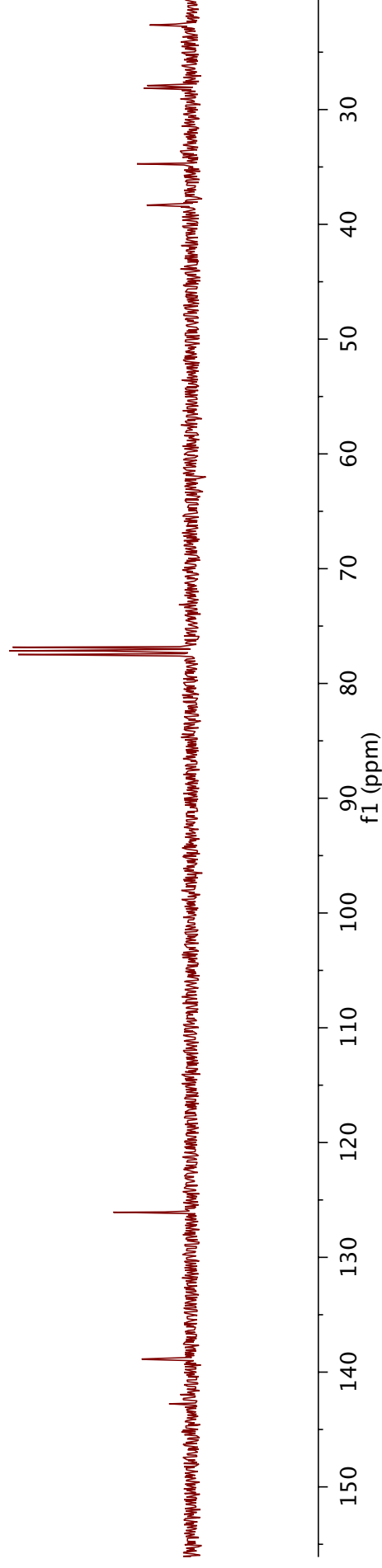
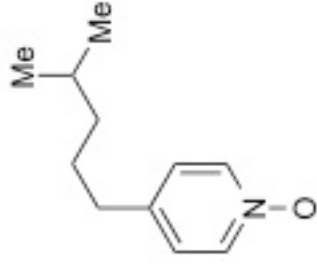
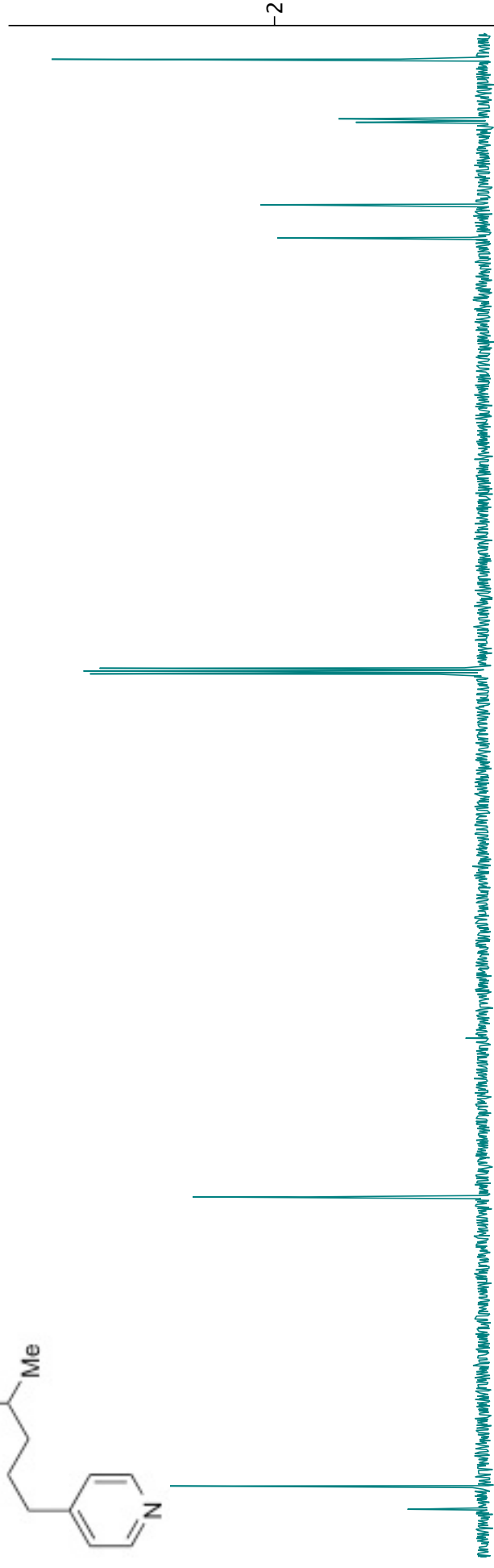
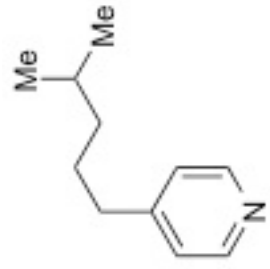


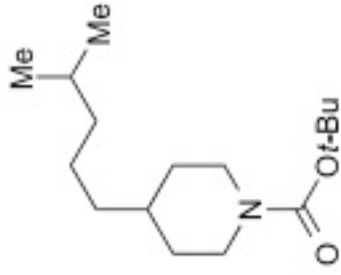
—142.76
—138.87
—126.07

77.48 CDCl₃
77.16 CDCl₃
76.84 CDCl₃

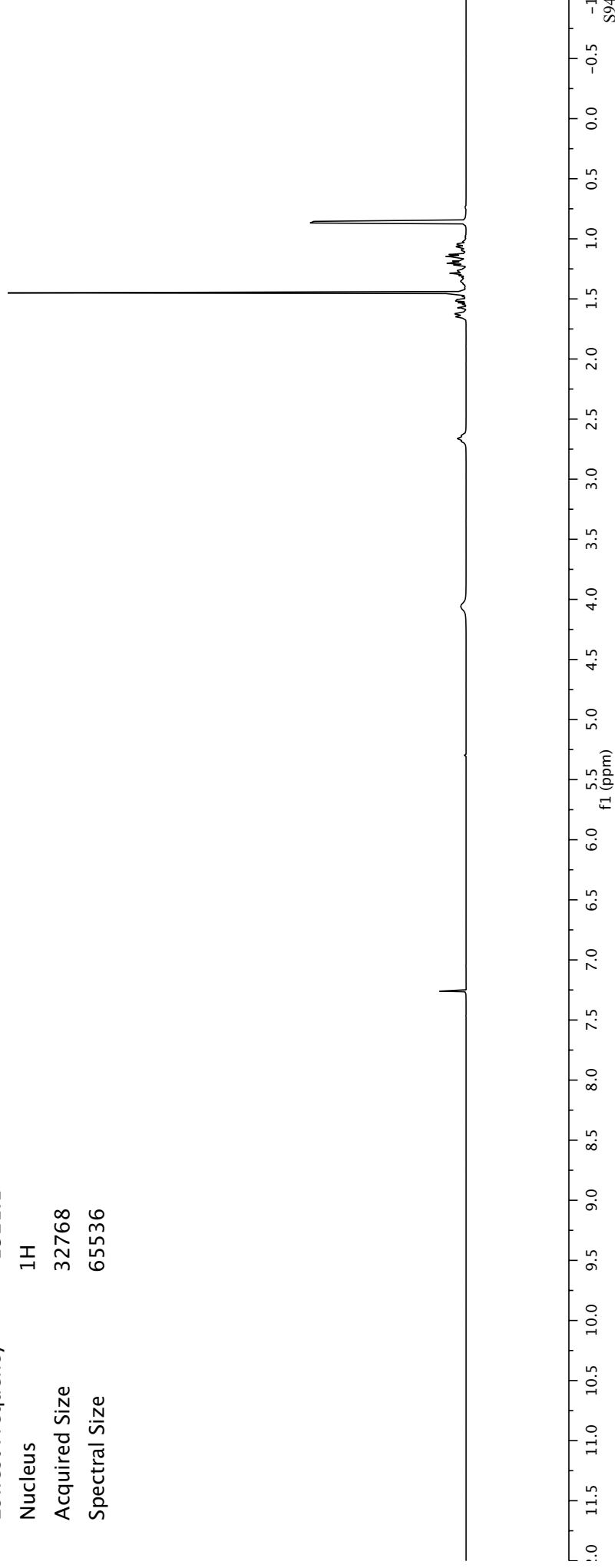
38.33
34.73
28.14
27.91
22.63

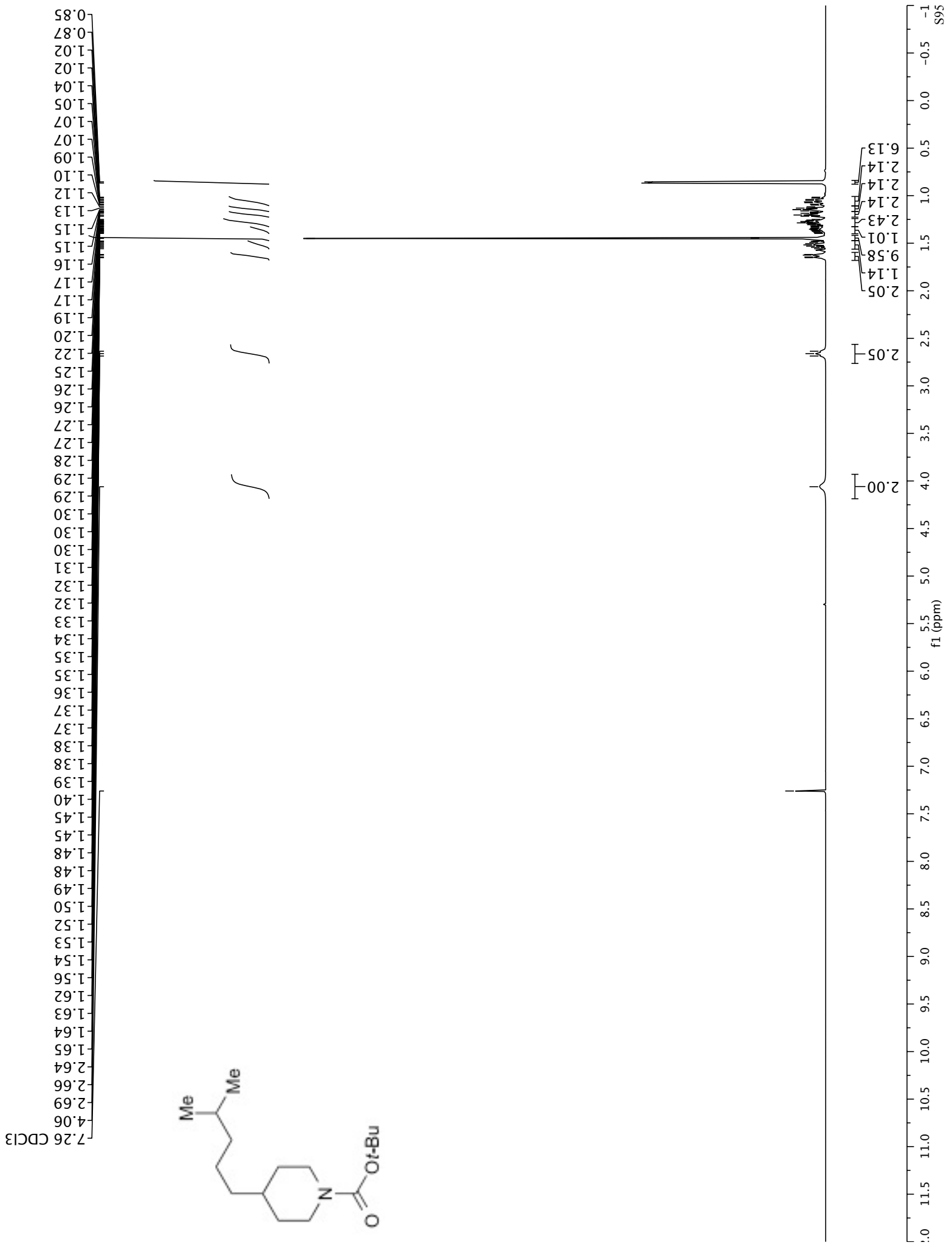
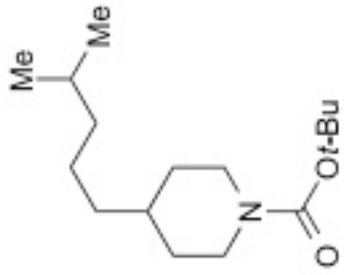


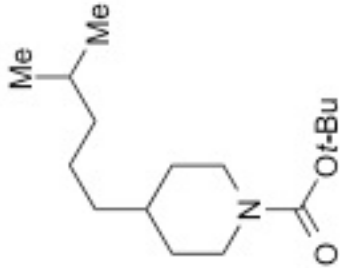




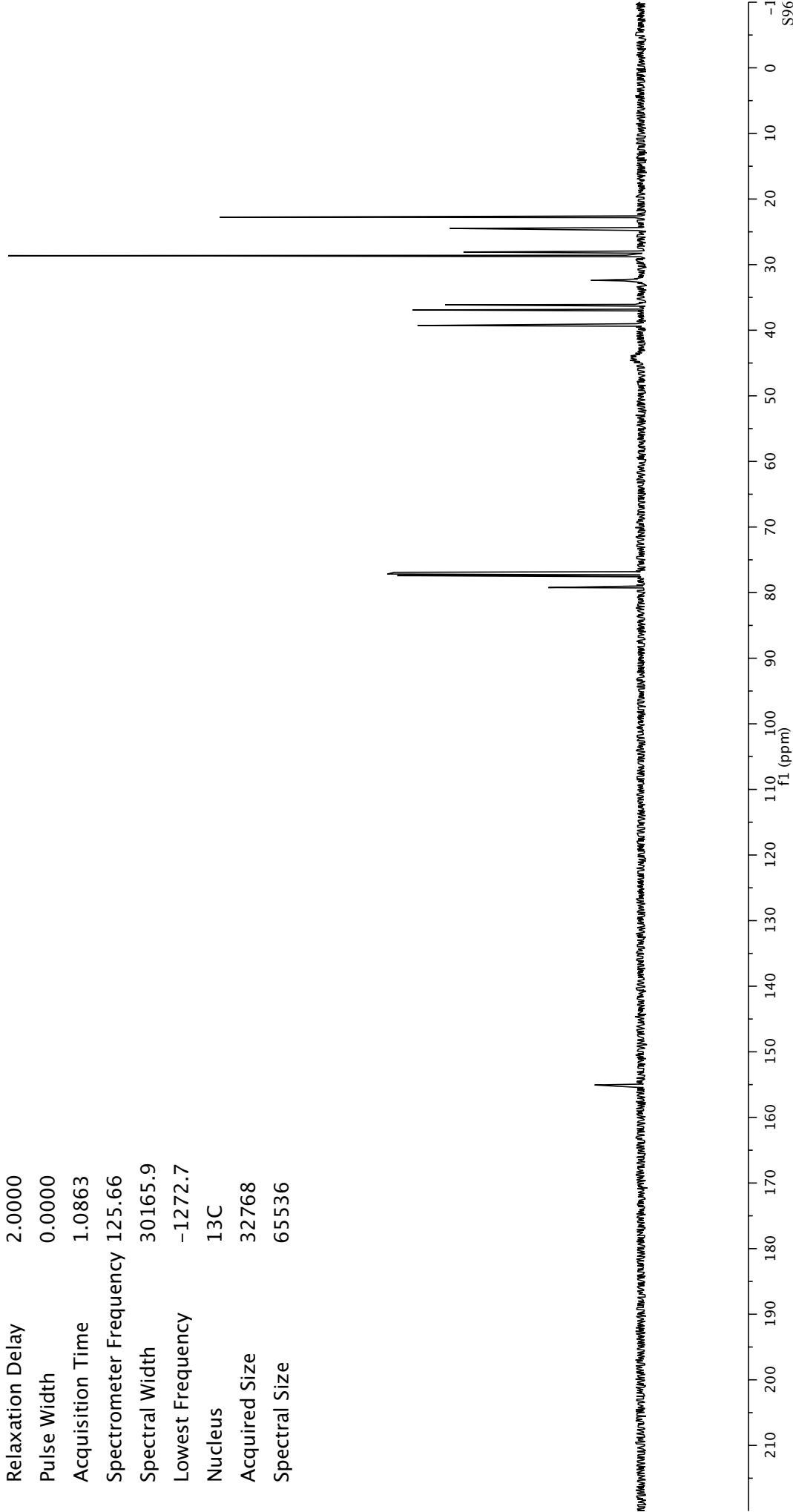
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	38
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1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

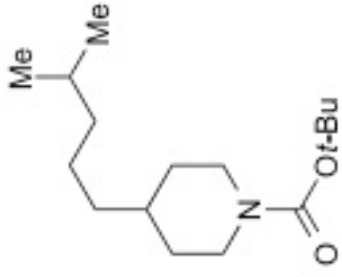






Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	635
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1272.7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

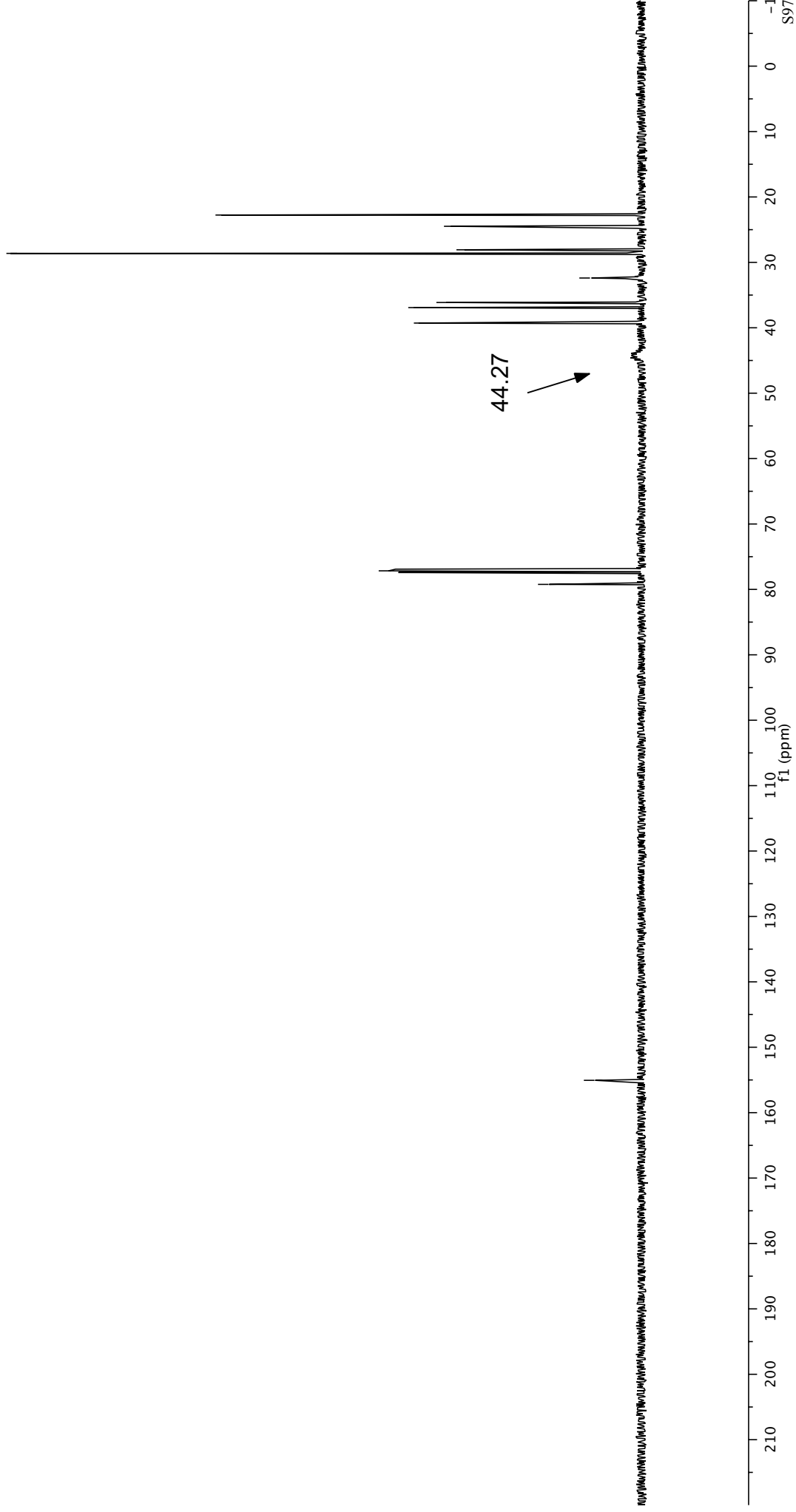


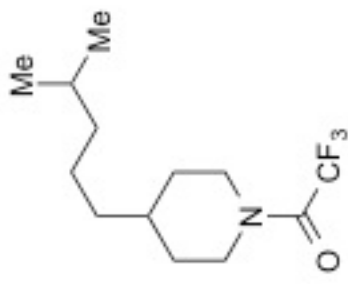


— 155.06

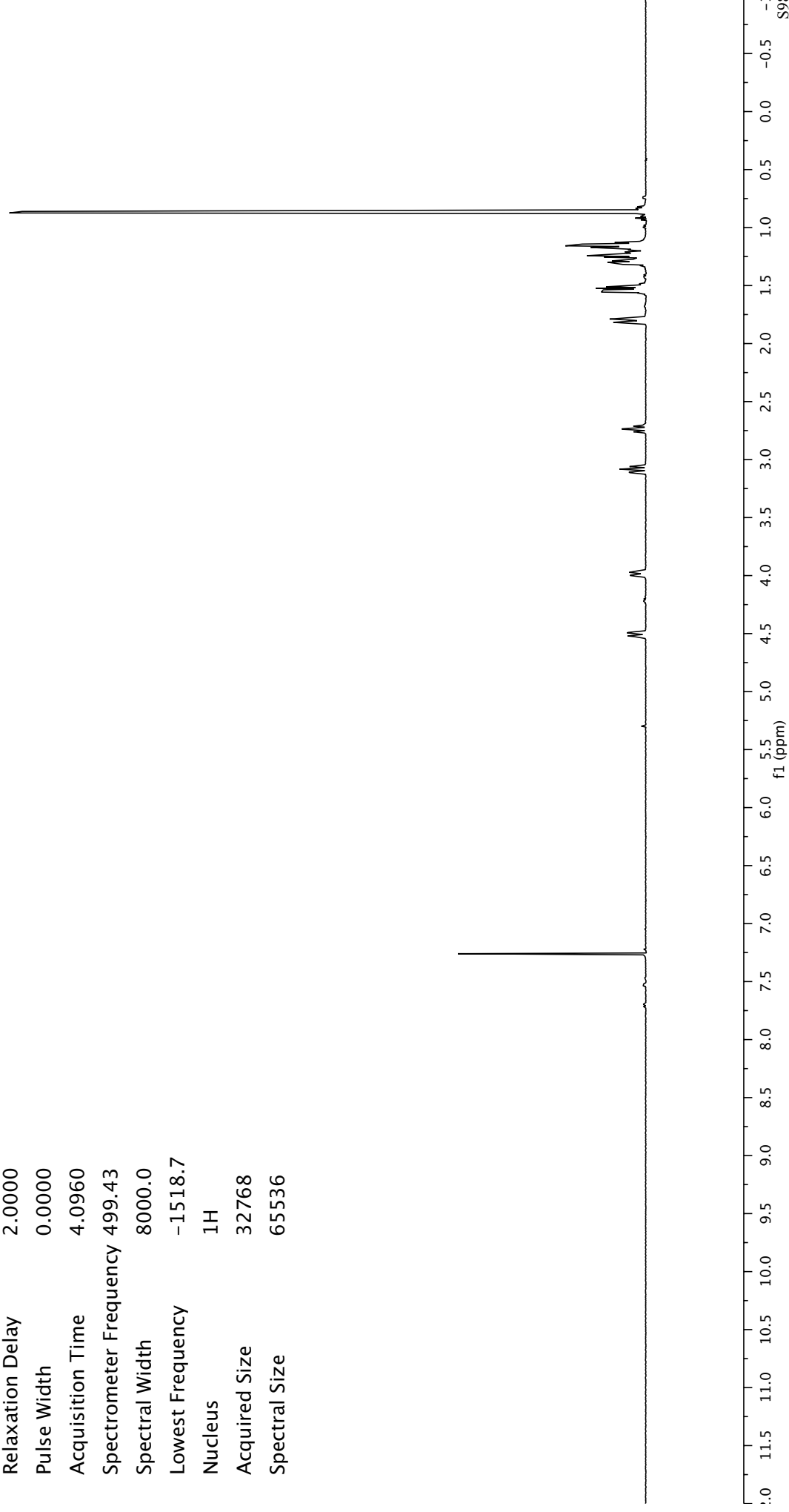
~ 79.23
~ 77.16 CDCl₃

39.28
36.92
36.13
32.39
28.63
28.08
24.49
22.76



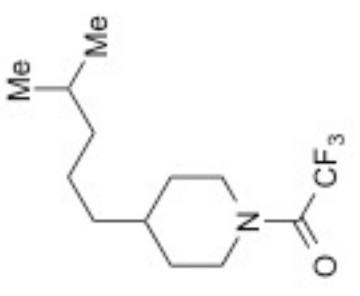


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Number of Scans	16
Receiver Gain	54
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	499.43
Spectral Width	8000.0
Lowest Frequency	-1518.7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

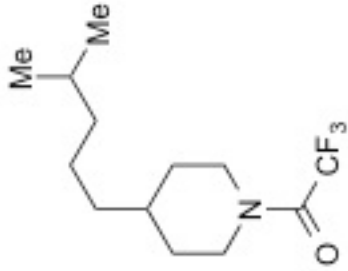


1.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1 S99

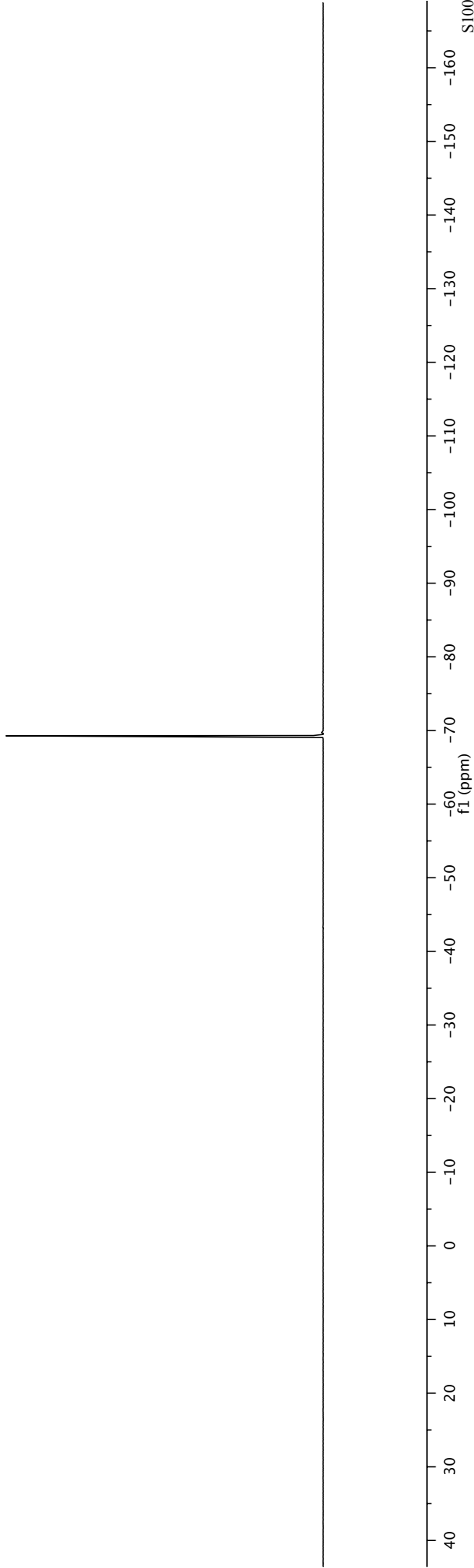
6.17 H
3.93 H
2.28 H
2.11 H
2.31 H
2.01 H
1.01 H
1.00 H
1.00 H

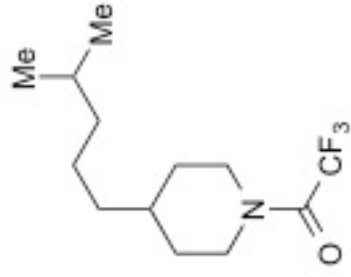


7.26 CDCl3
4.53
4.52
4.52
4.50
4.49
4.00
3.97
3.11
3.11
3.09
3.09
3.08
3.06
3.06
2.74
2.74
2.73
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0.86

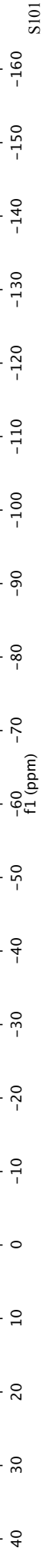


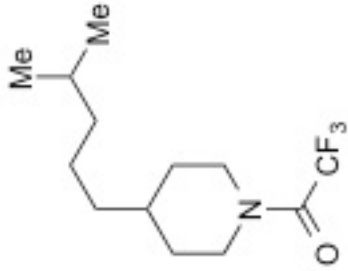
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	132
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency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



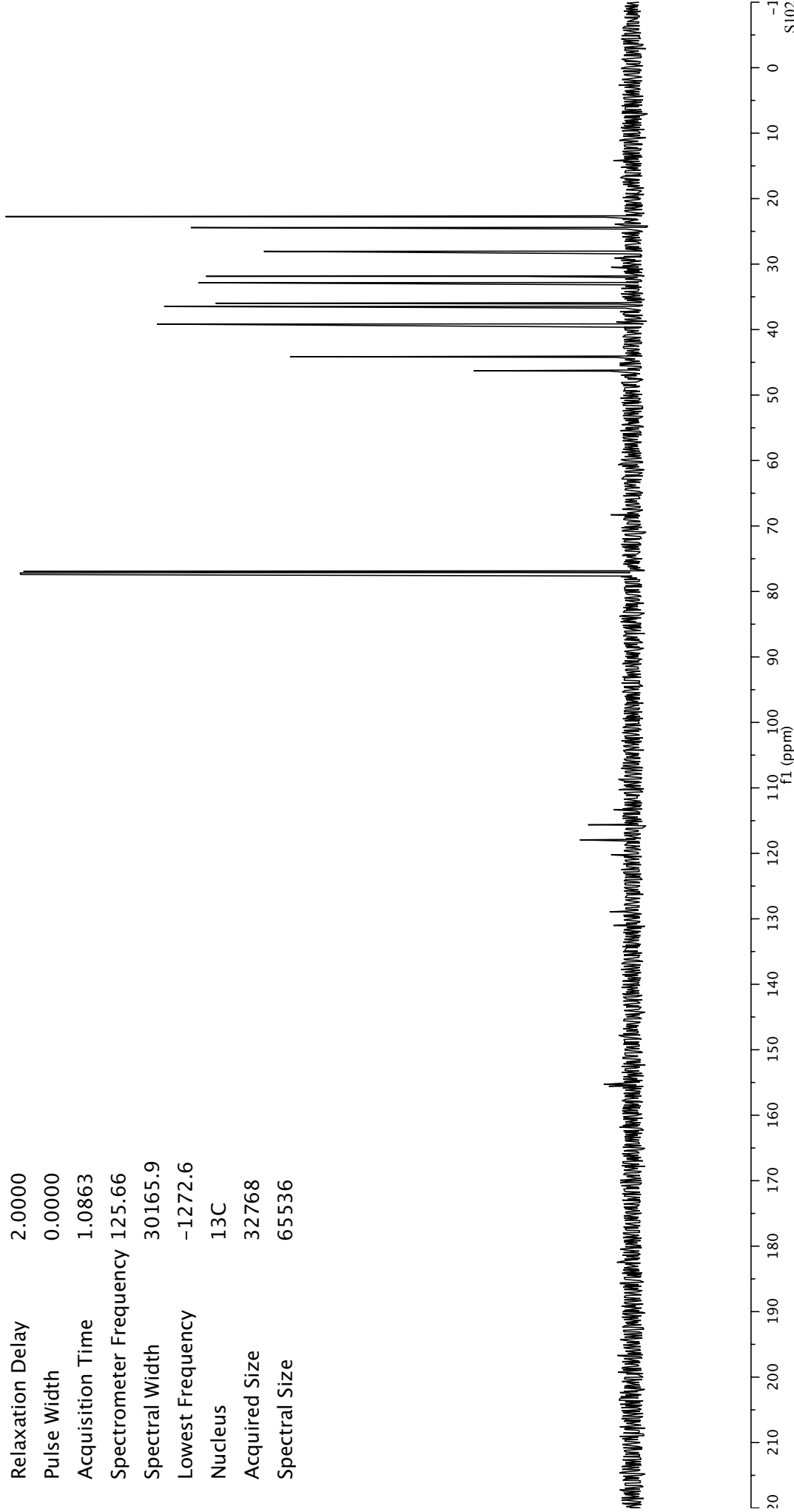


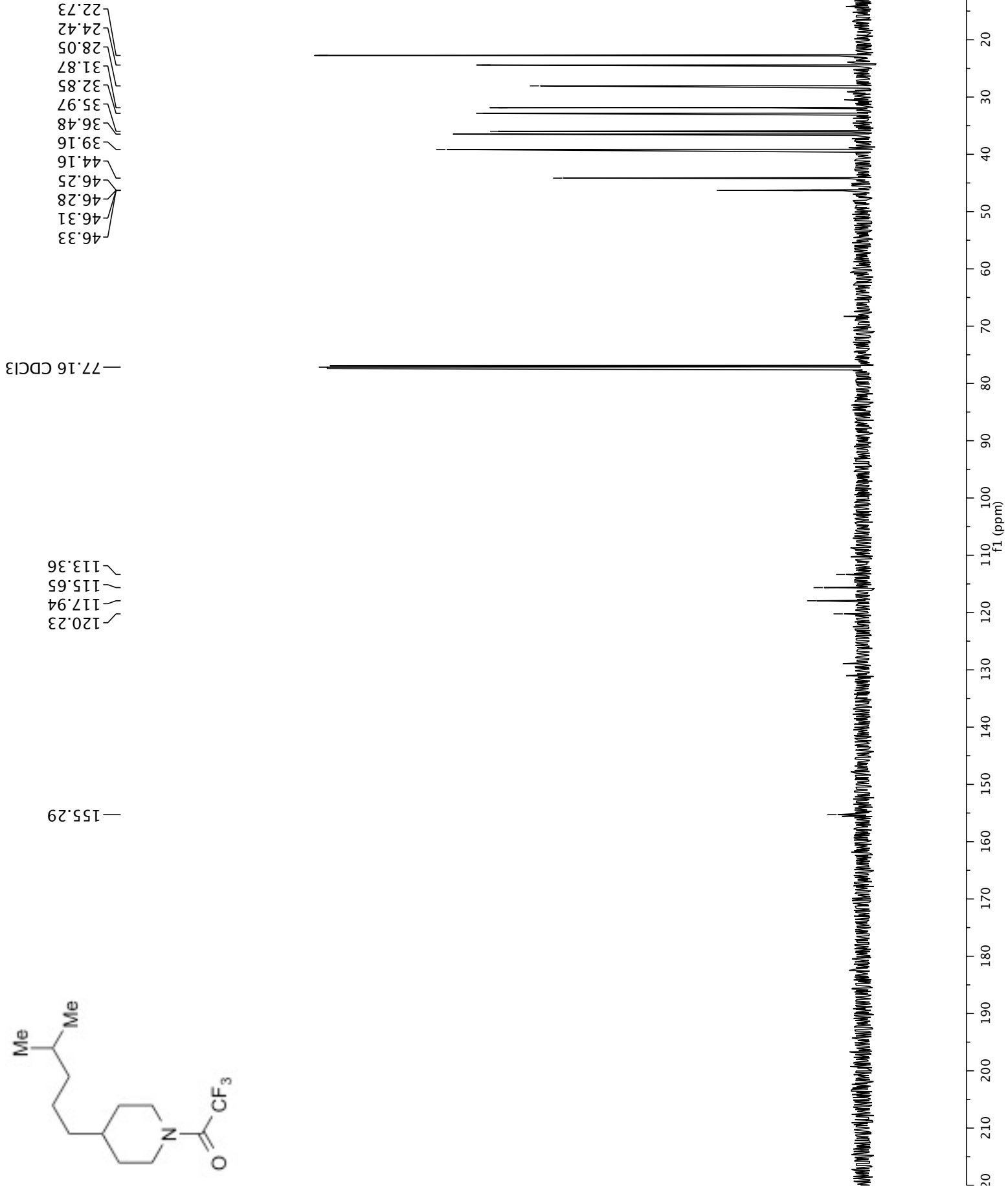
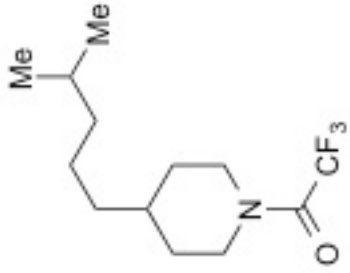
—-69.27

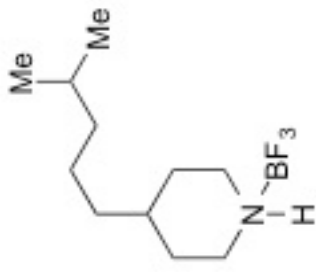




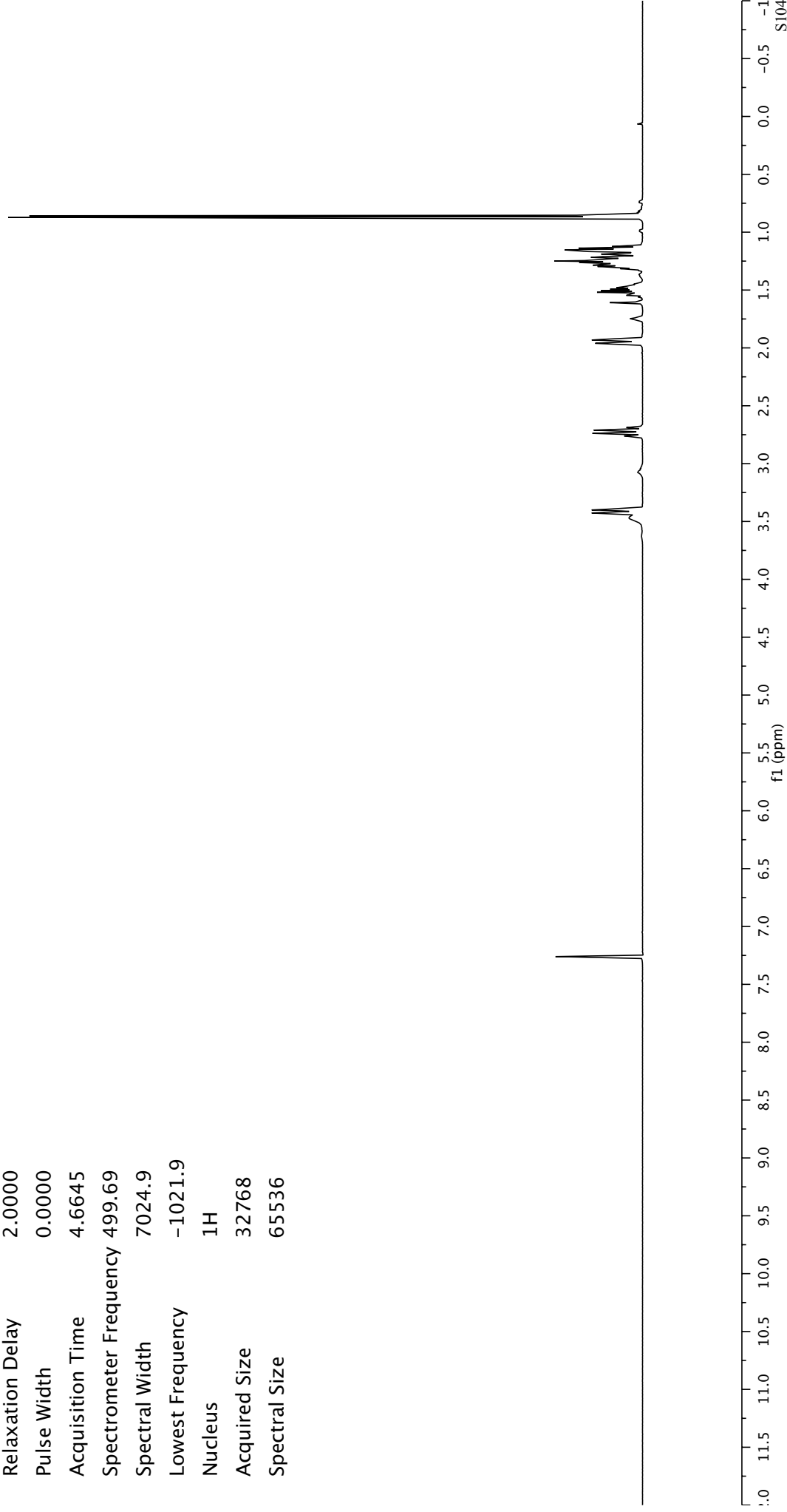
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	732
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1272.6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

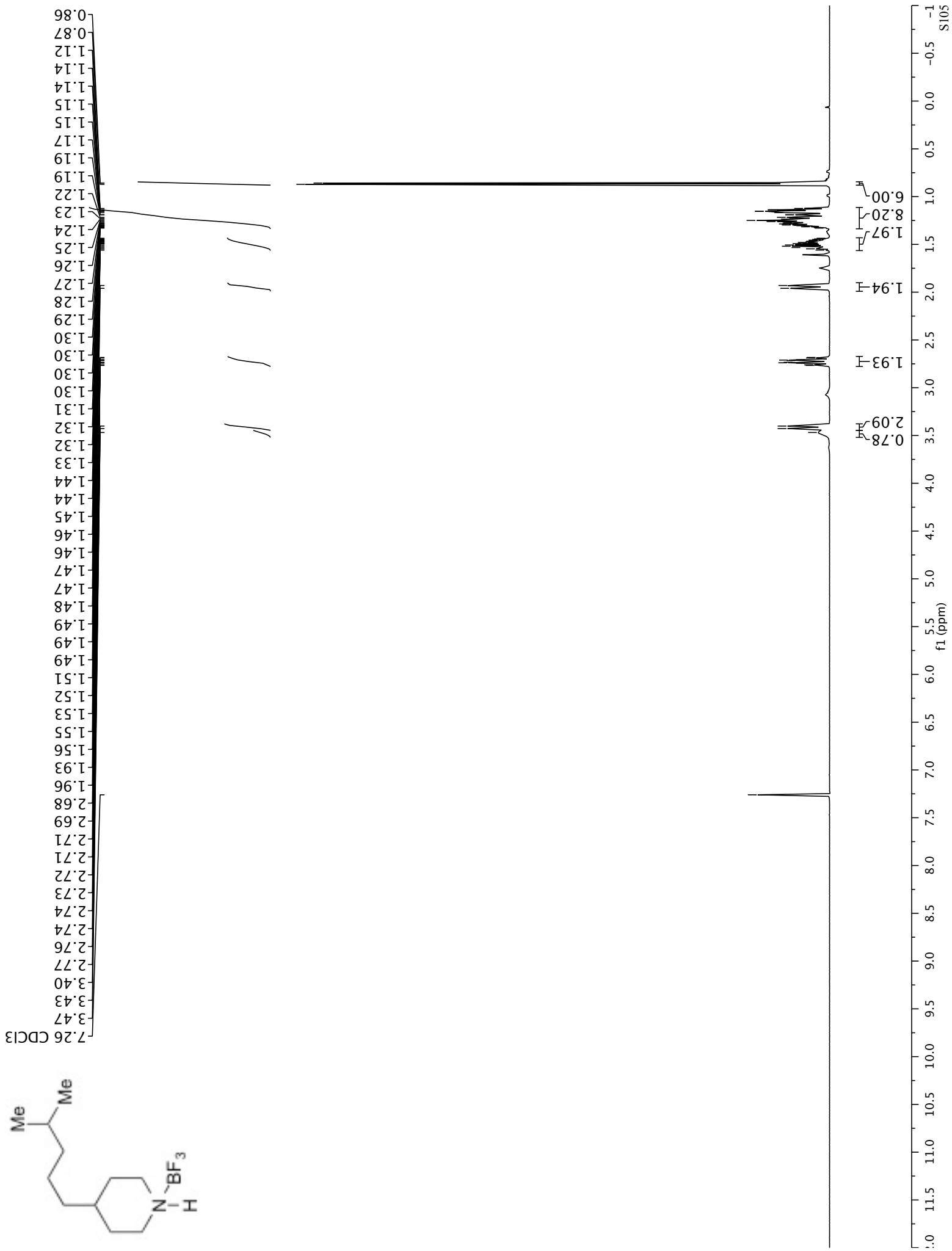
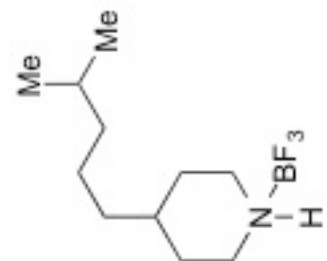


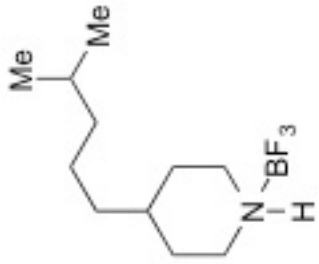




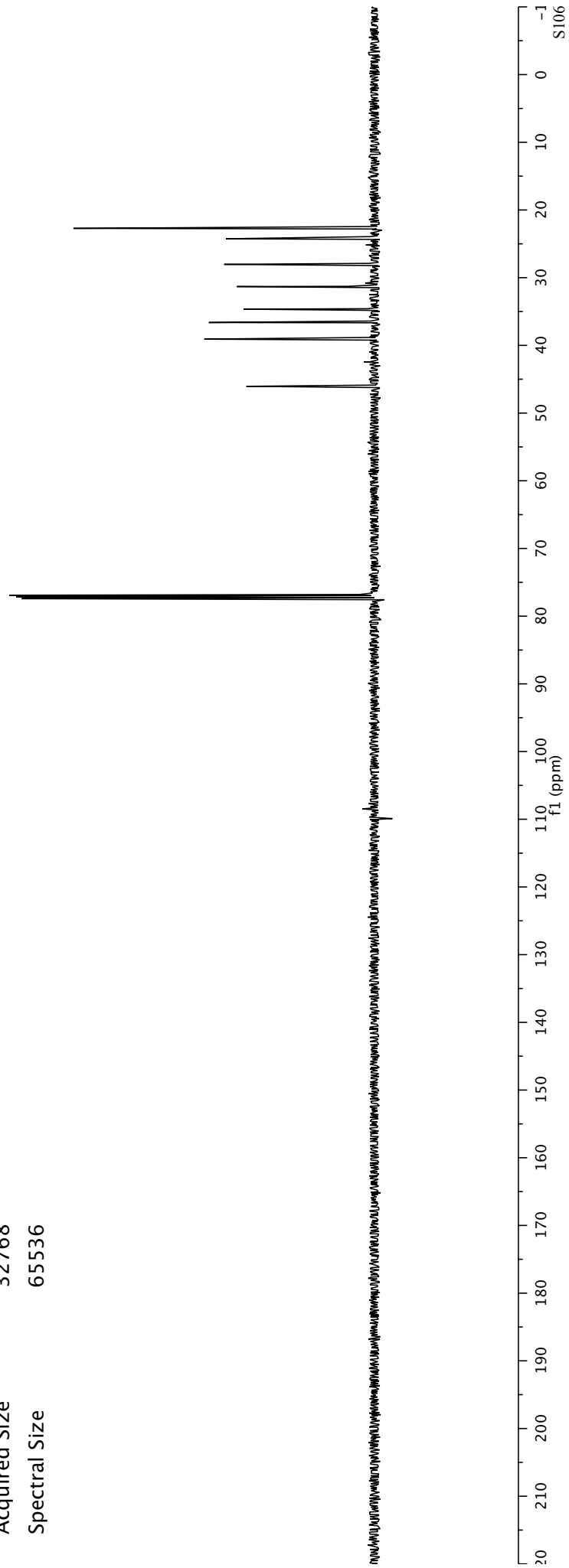
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	16
Receiver Gain	46
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.69
Spectral Width	7024.9
Lowest Frequency	-1021.9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

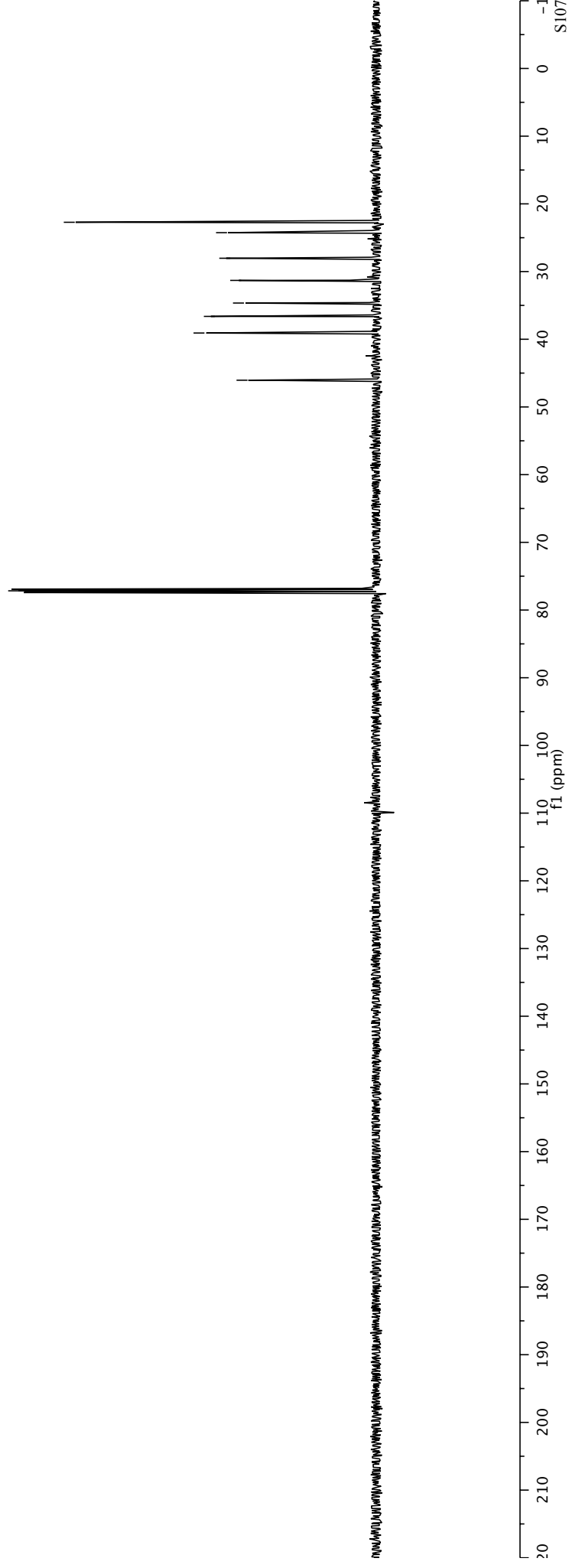
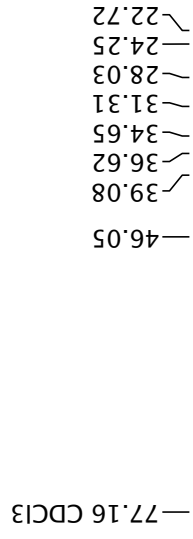
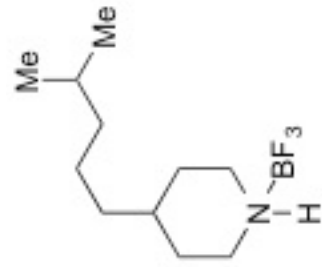


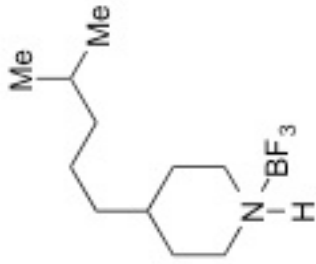




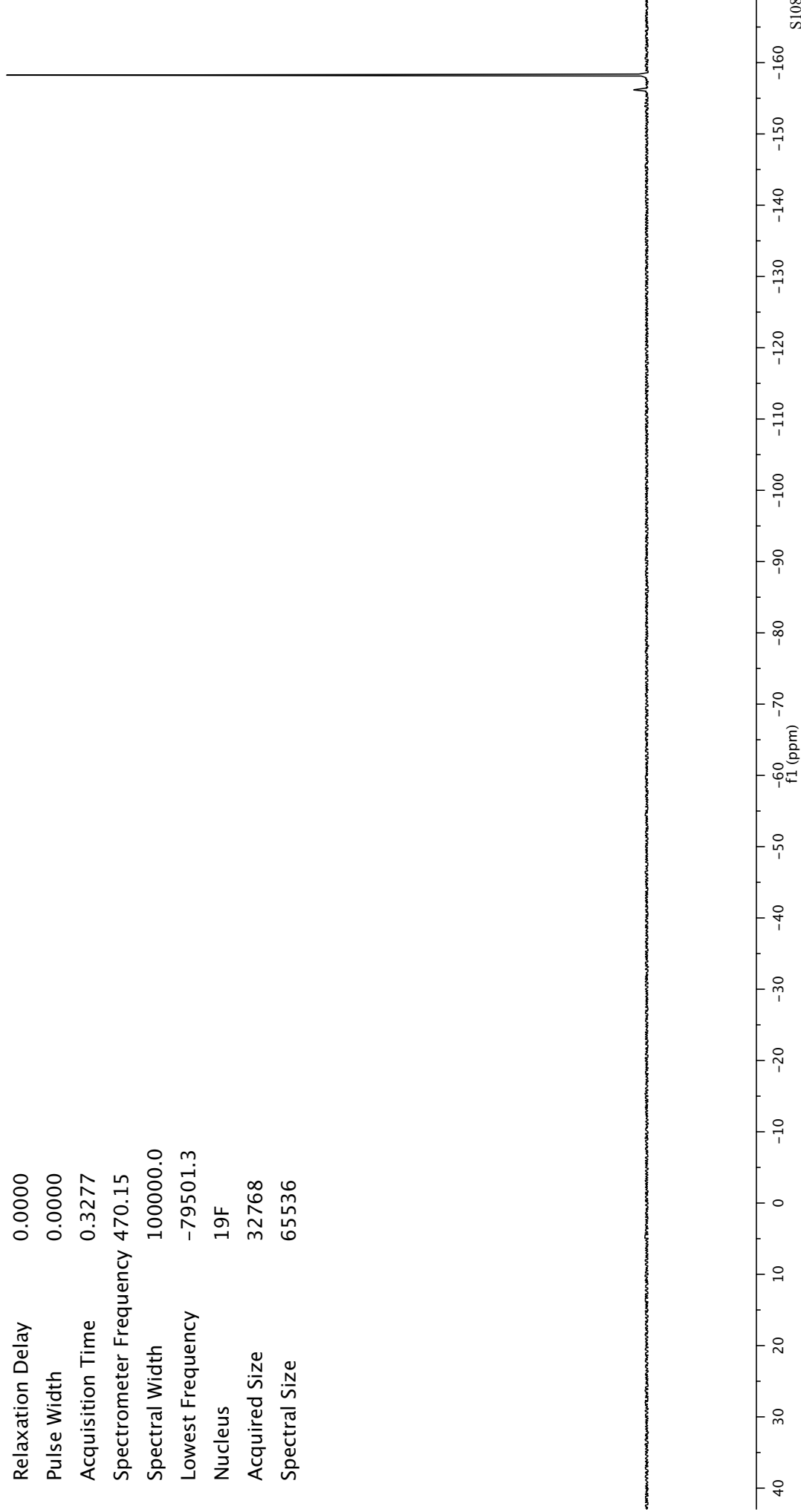
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	1012
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1272.5
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

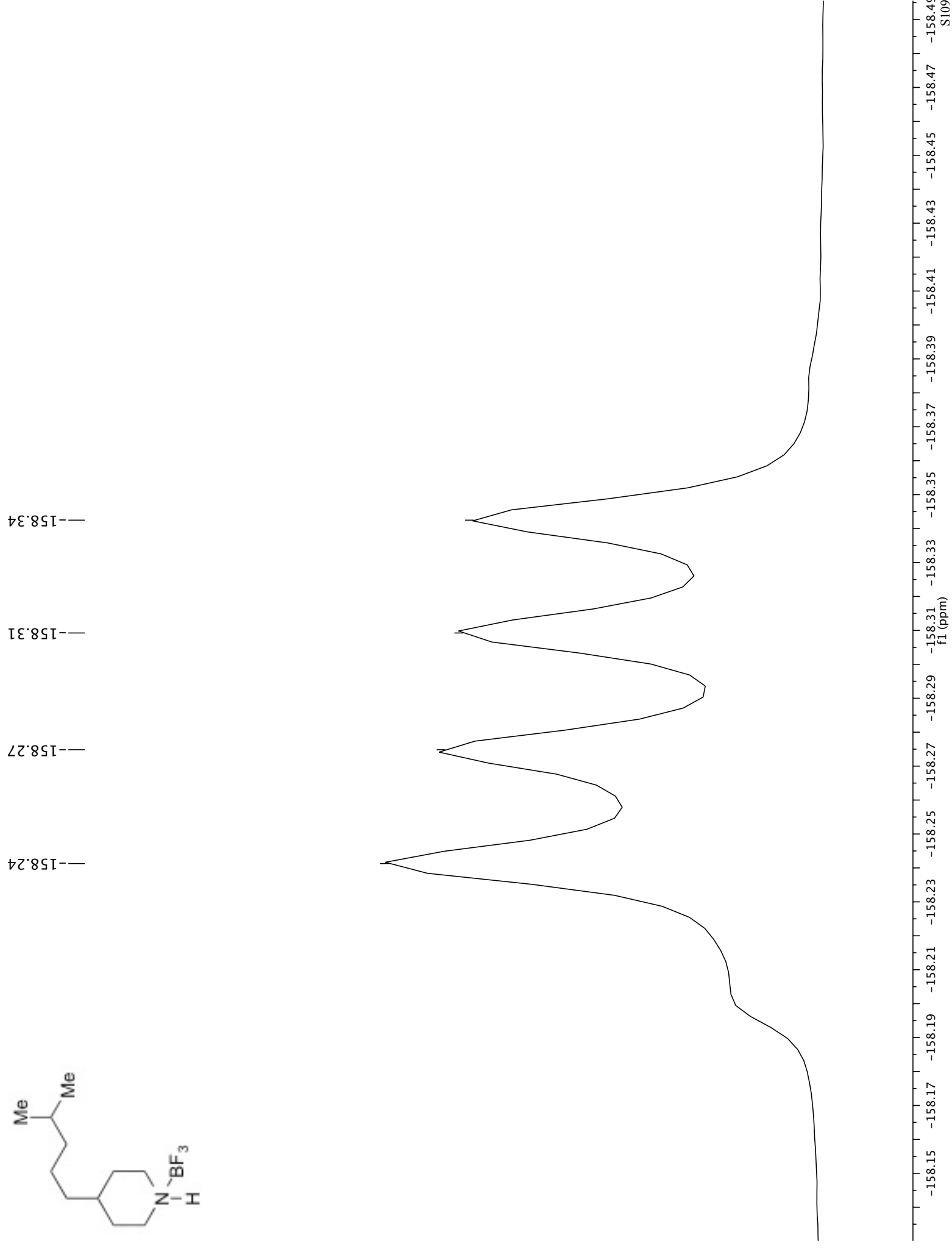
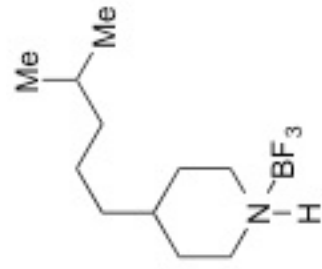






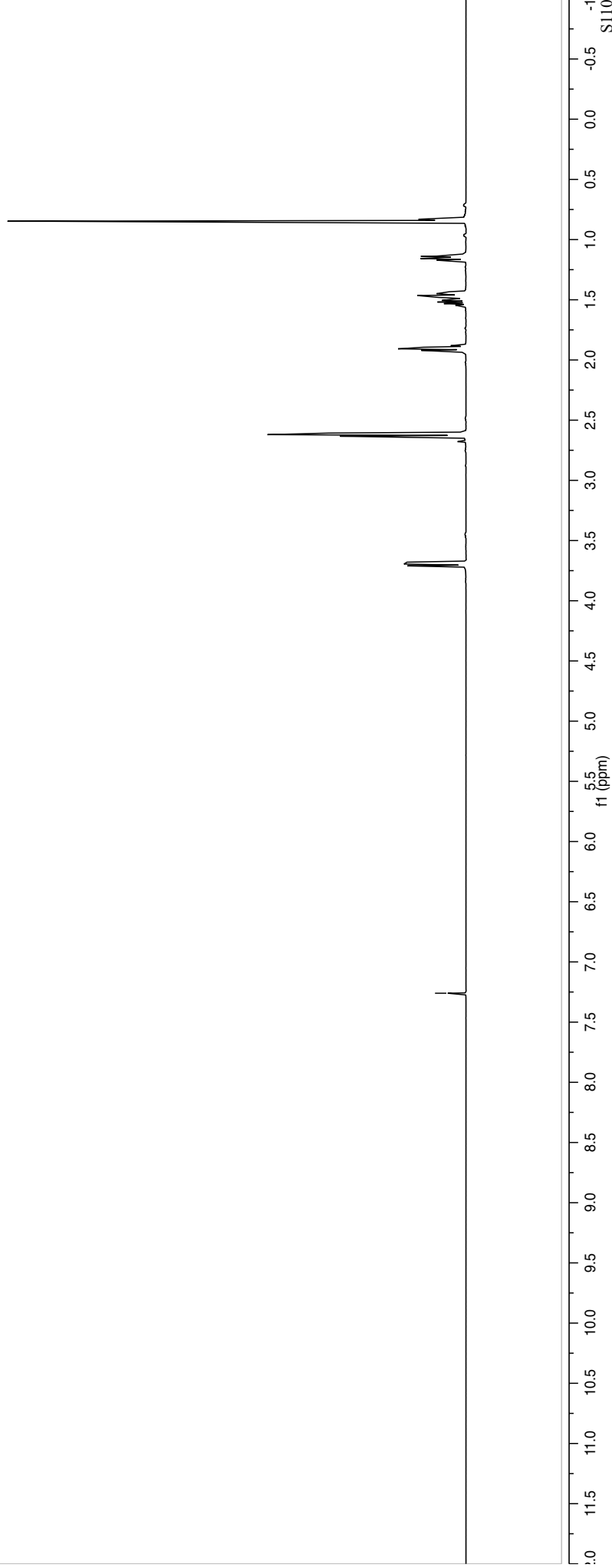
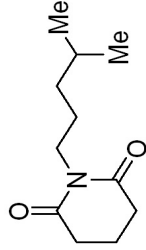
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	132
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency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



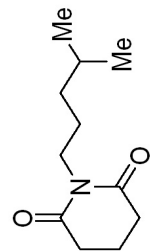


7.26 CDCl3

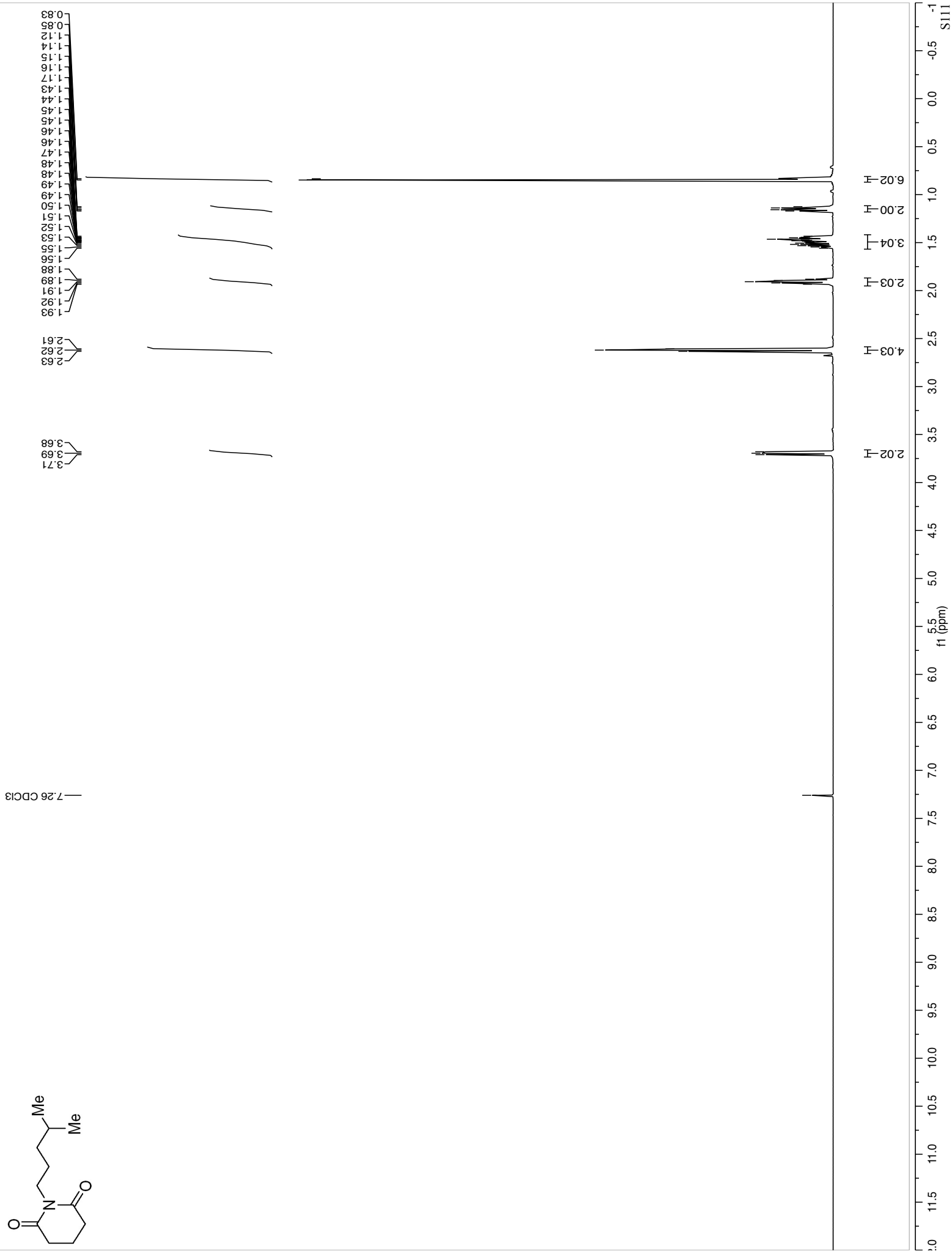
Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	8
9 Receiver Gain	41
10 Relaxation Delay	0.0000
11 Pulse Width	0.0000
12 Acquisition Time	4.6645
13 Spectrometer Frequency	499.69
14 Spectral Width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



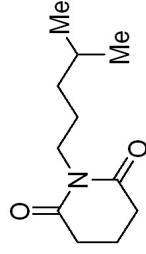
S110



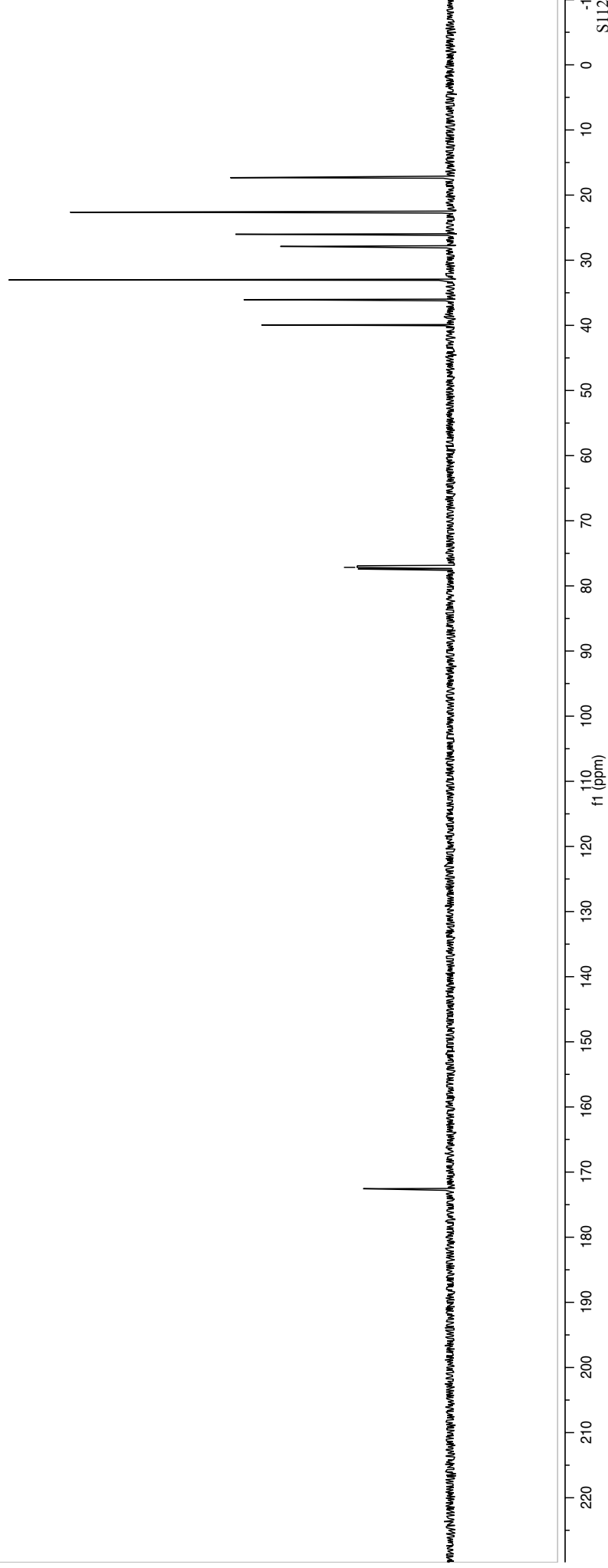
7.26 CDCl₃

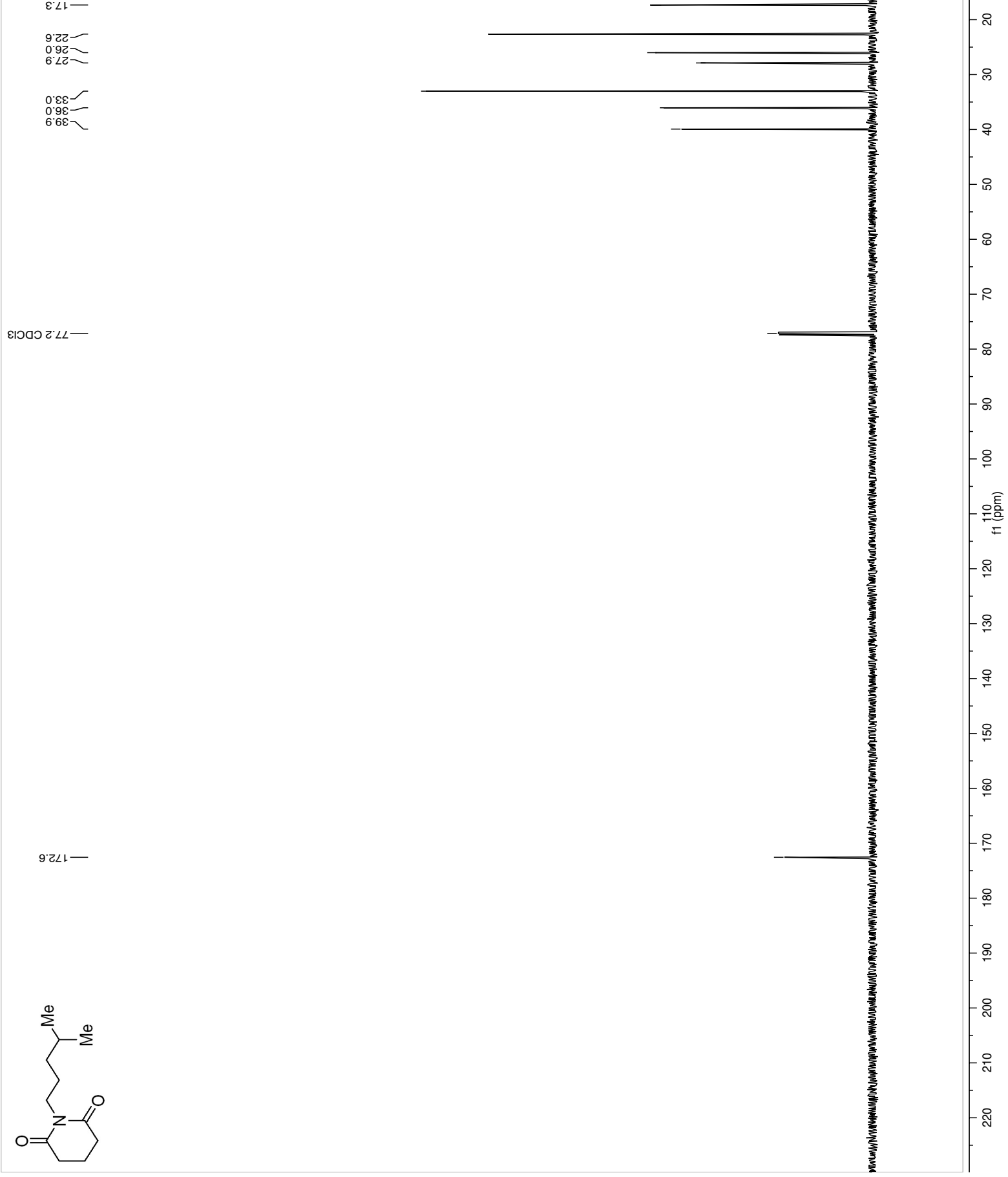
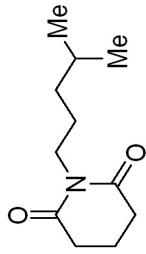


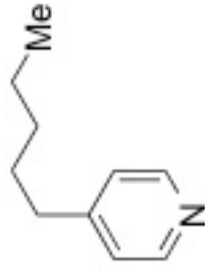
— 77.2 CDCl₃



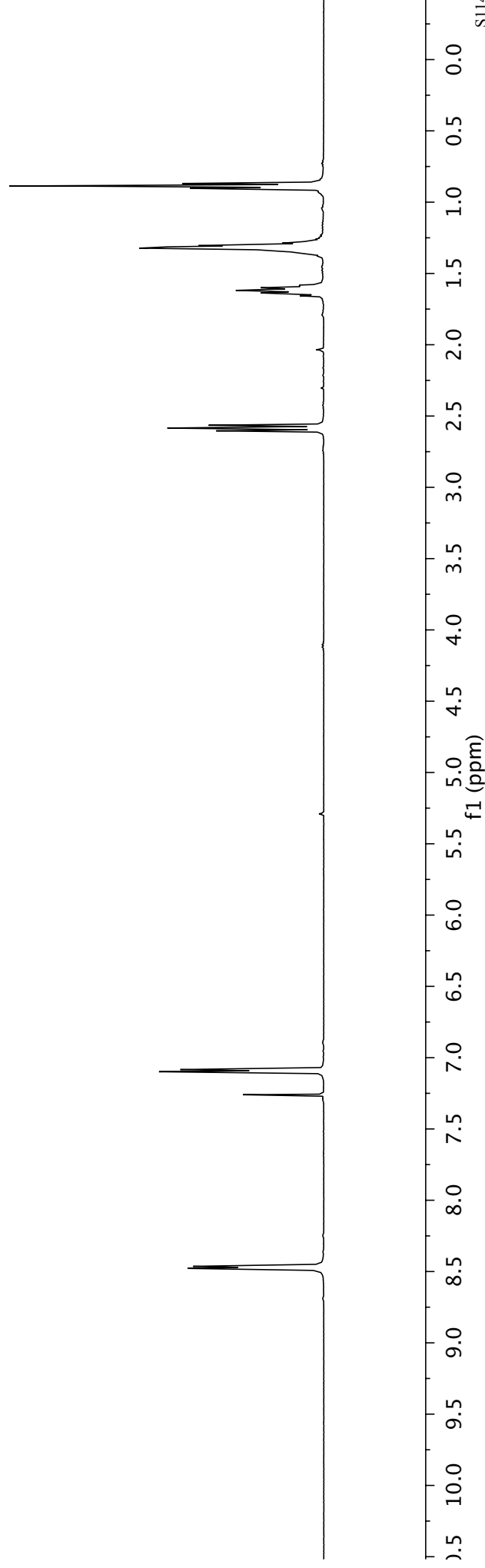
Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl ₃
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	80
9 Receiver Gain	60
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.0863
13 Spectrometer Frequency	125.66
14 Spectral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

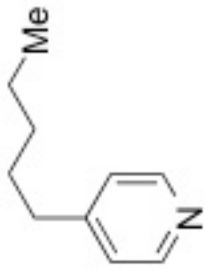






Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	5mmsw
Receiver Gain	52
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	399.74
Spectral Width	8000.0
Lowest Frequency	-2421.6
Nucleus	1H
Acquired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

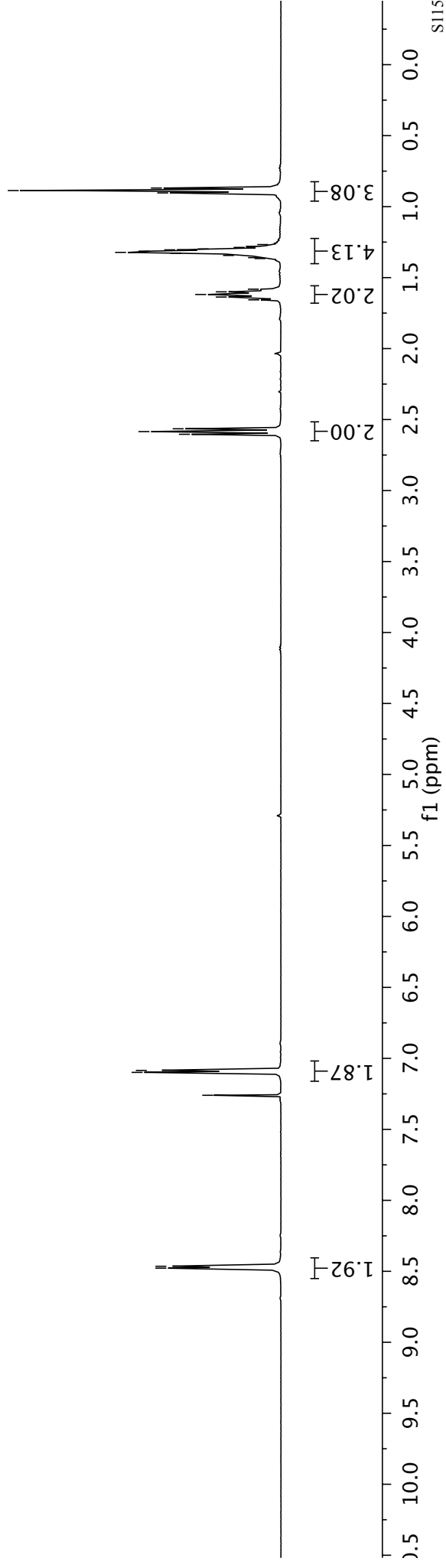
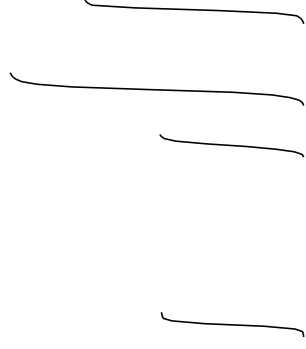


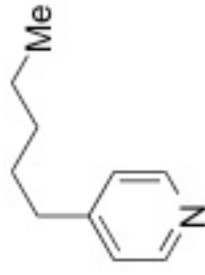


7.26 CDCl₃
7.10
7.08

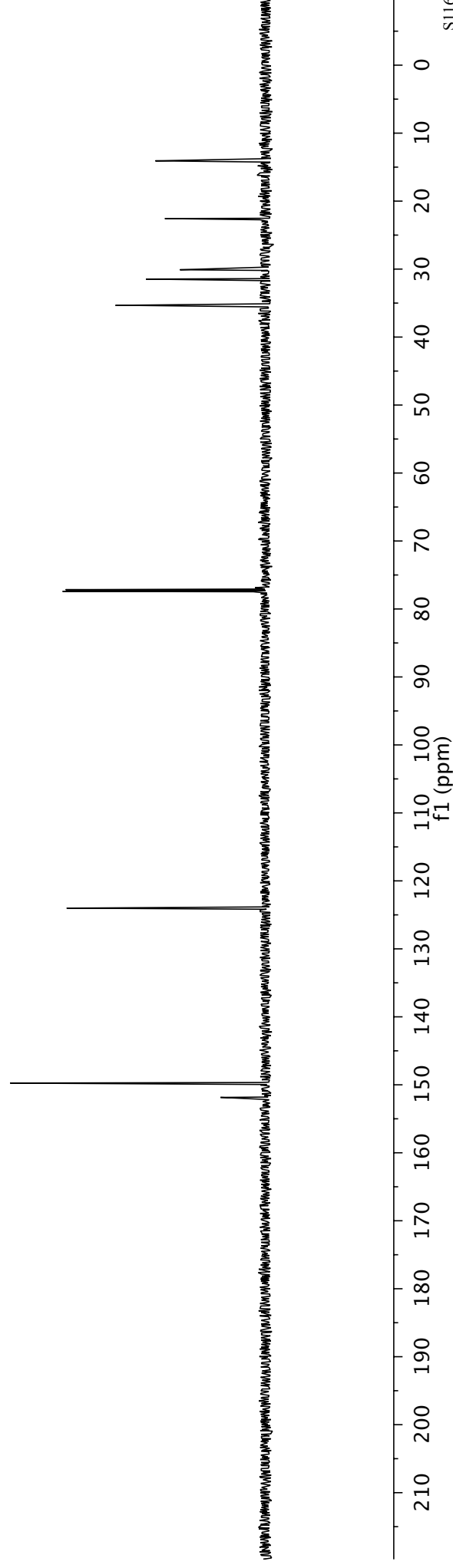
8.48
8.46

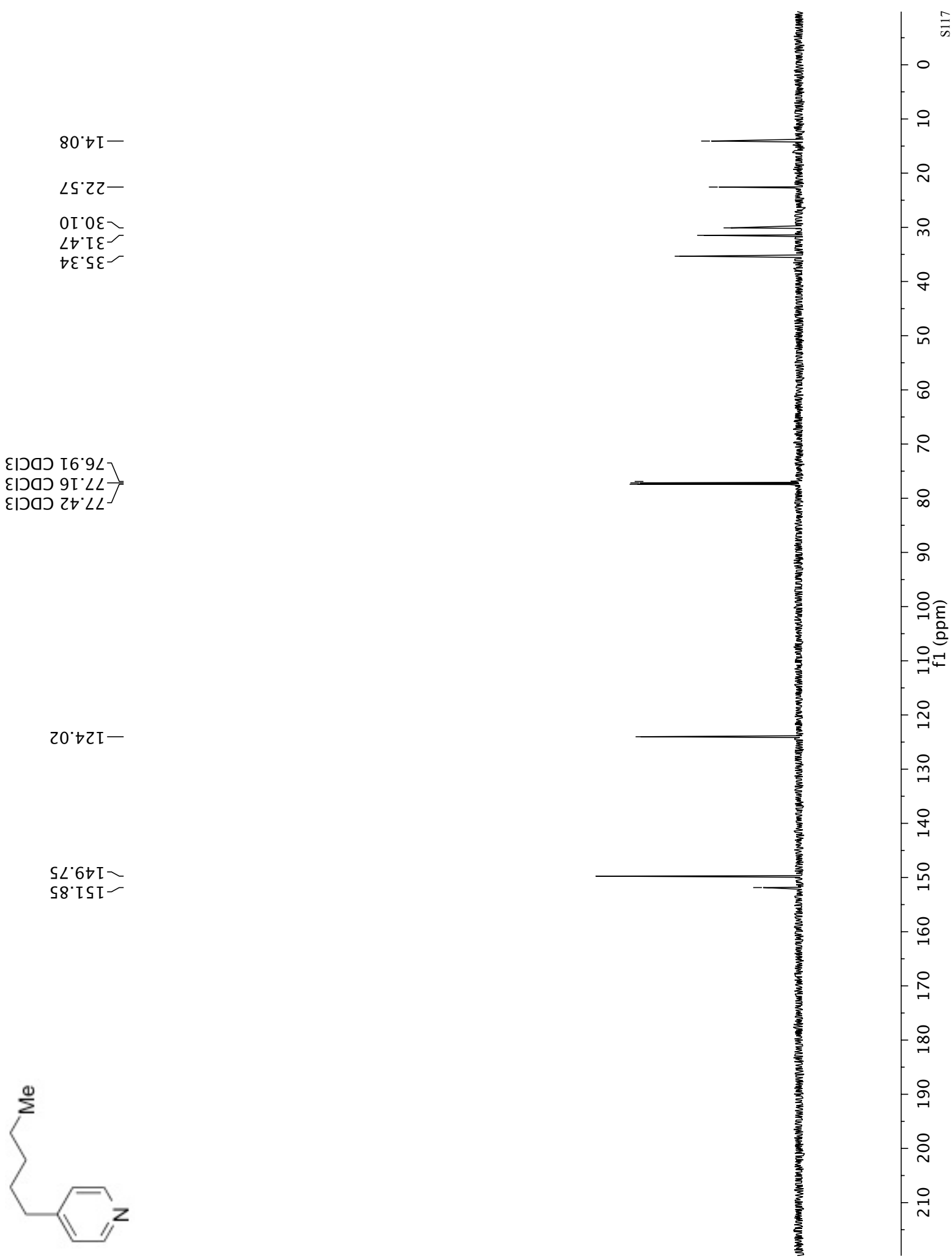
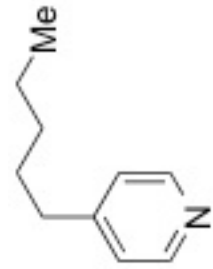
2.60
2.58
2.56
1.66
1.64
1.62
1.60
1.58
1.37
1.36
1.34
1.33
1.32
1.31
1.30
1.30
1.29
1.28
1.27
0.90
0.89
0.87



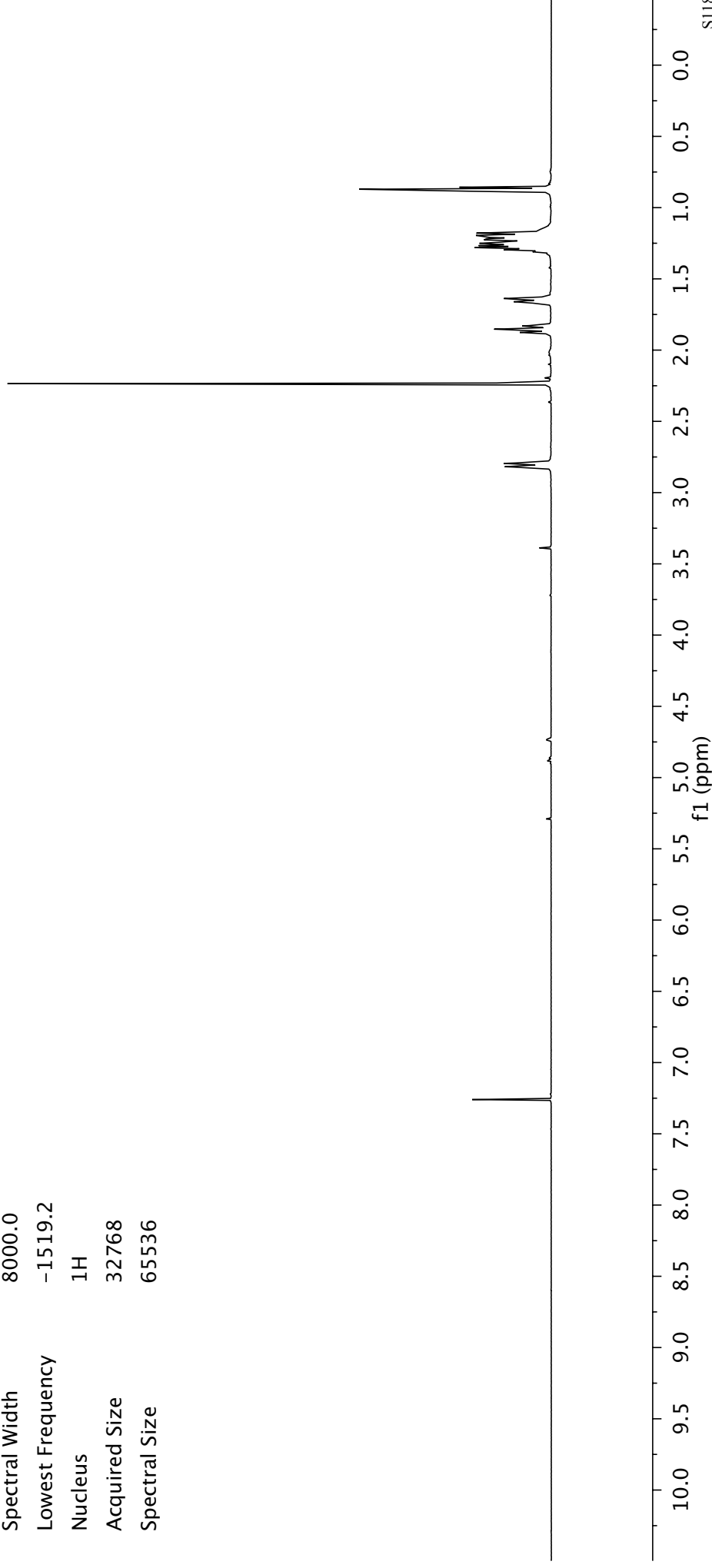
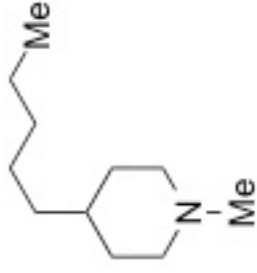


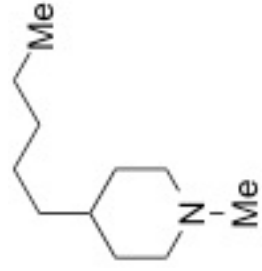
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2200.5
Nucleus	¹³ C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



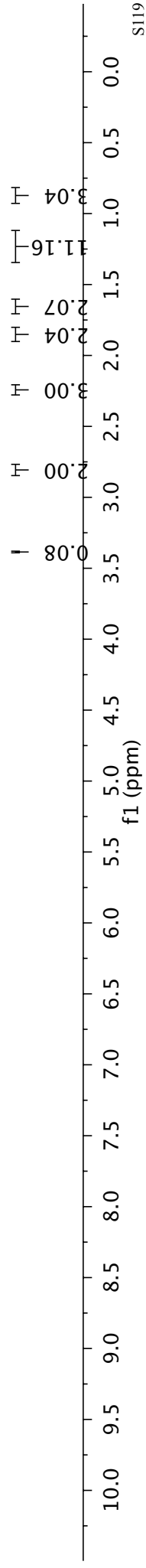
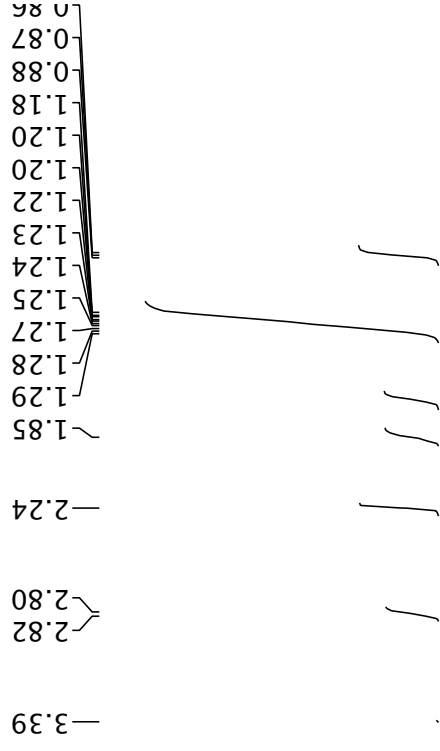


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	50
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	499.43
Spectral Width	8000.0
Lowest Frequency	-1519.2
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

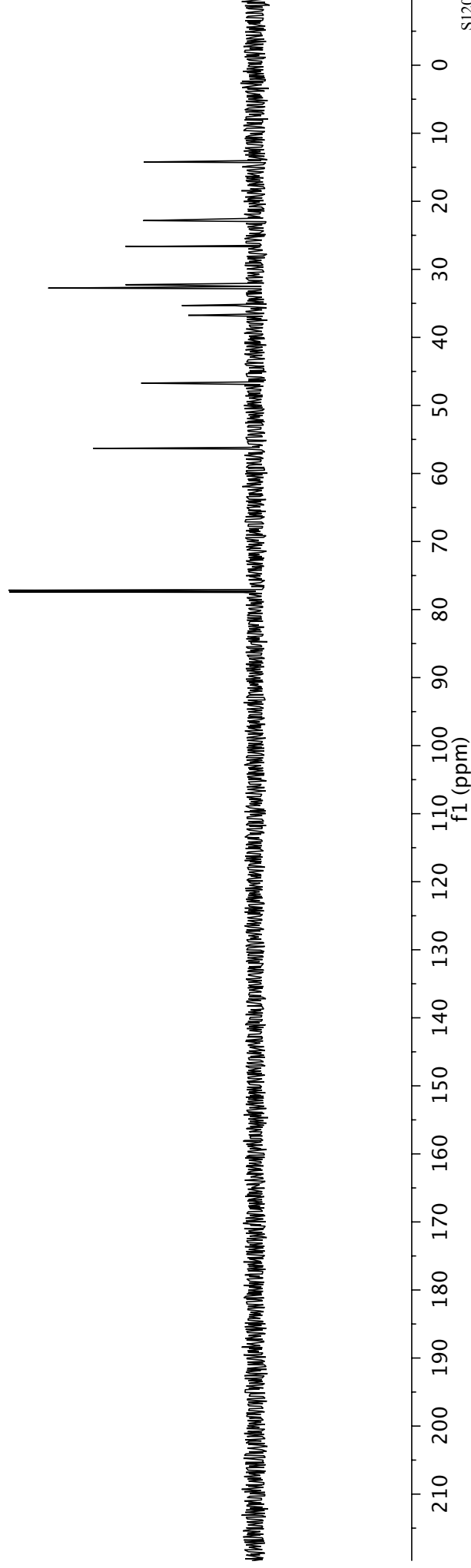
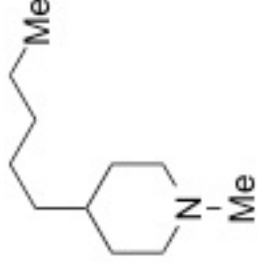


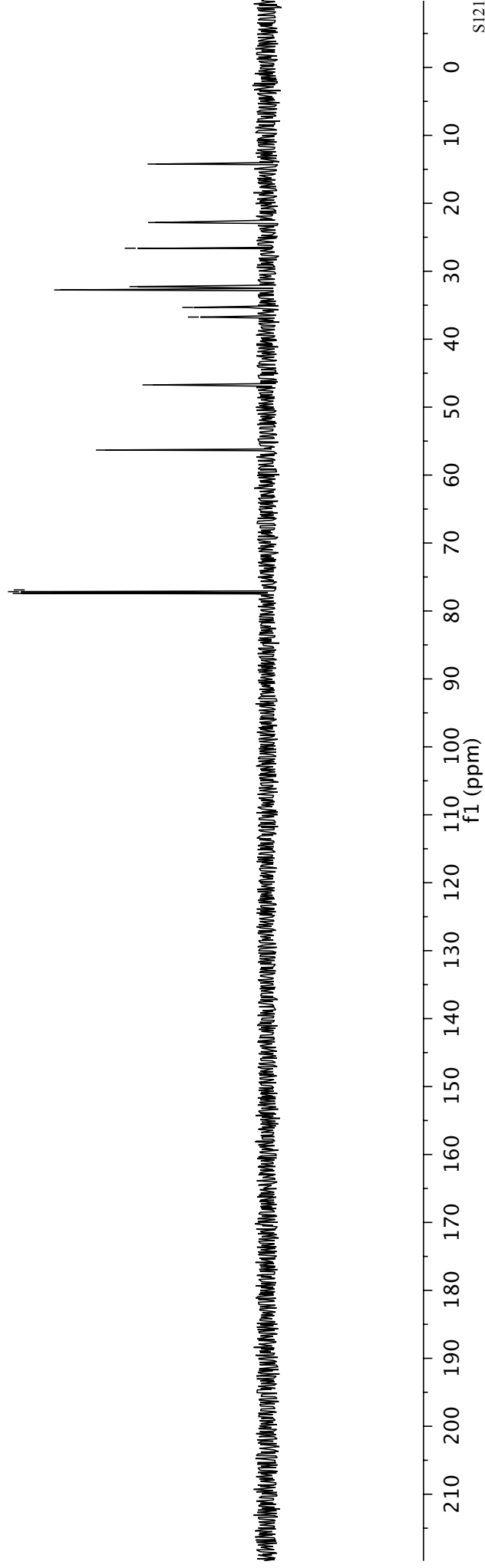
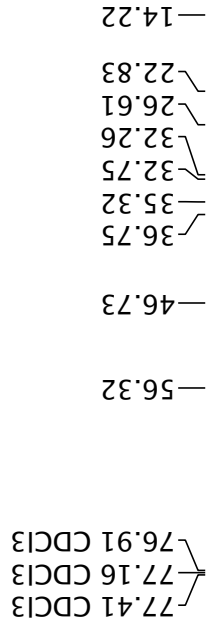
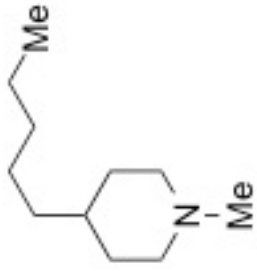


— 7.26 CDCl₃

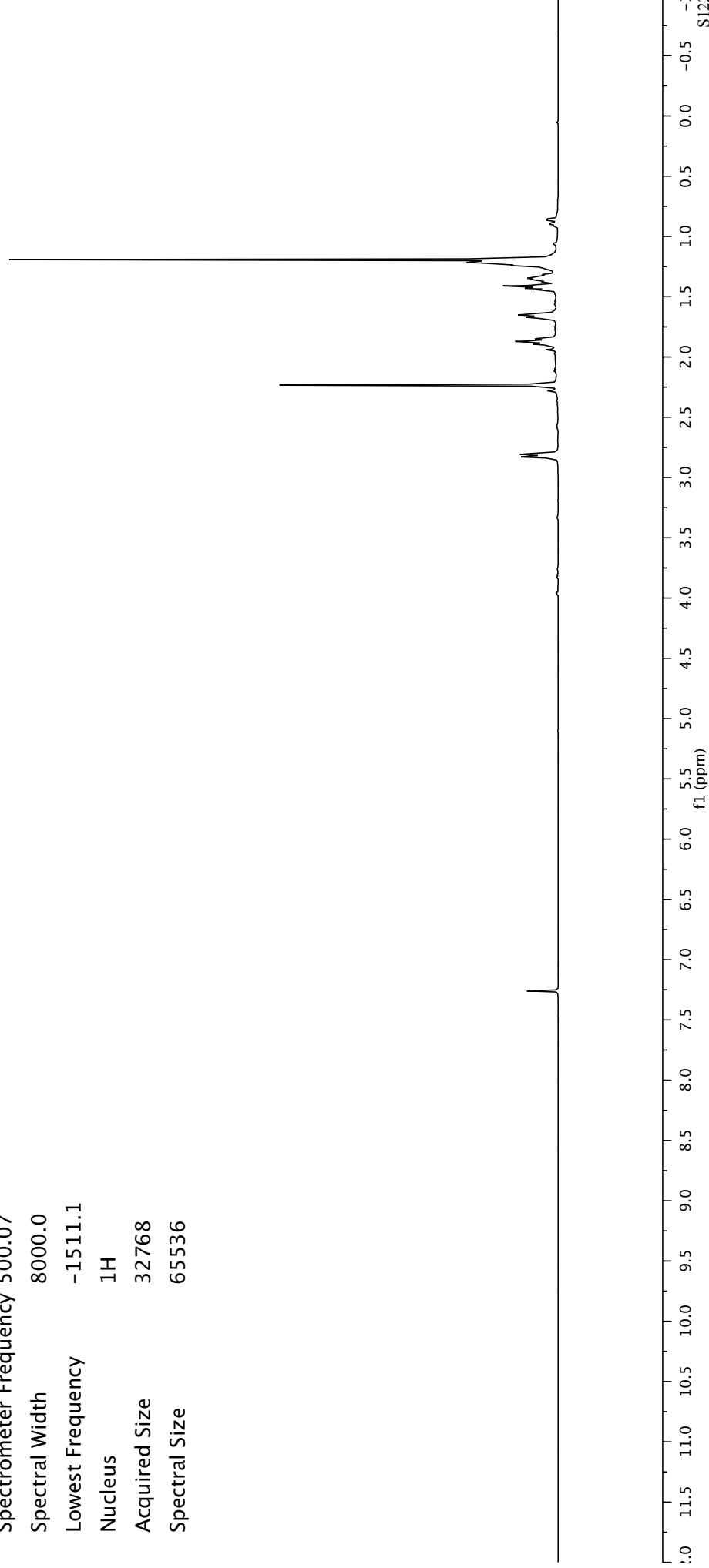
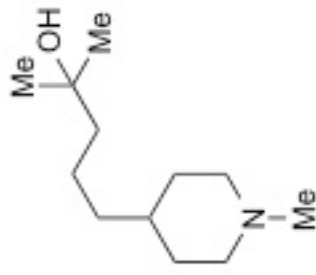


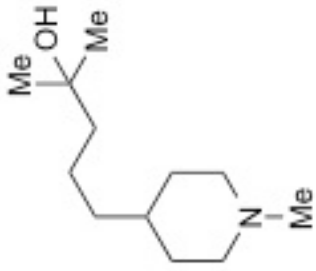
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2200.1
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536





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	1H
Acquired Size	32768
Spectral Size	65536





— 7.26 CDCl₃

2.83
2.82
2.81
2.80
2.23
1.89
1.88
1.87
1.85
1.67
1.65
1.44
1.44
1.43
1.42
1.42
1.41
1.40
1.38
1.38
1.37
1.36
1.36
1.35
1.34
1.34
1.33
1.33
1.33
1.32
1.27
1.27
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1.23
1.22
1.22
1.21
1.21
1.19
1.19

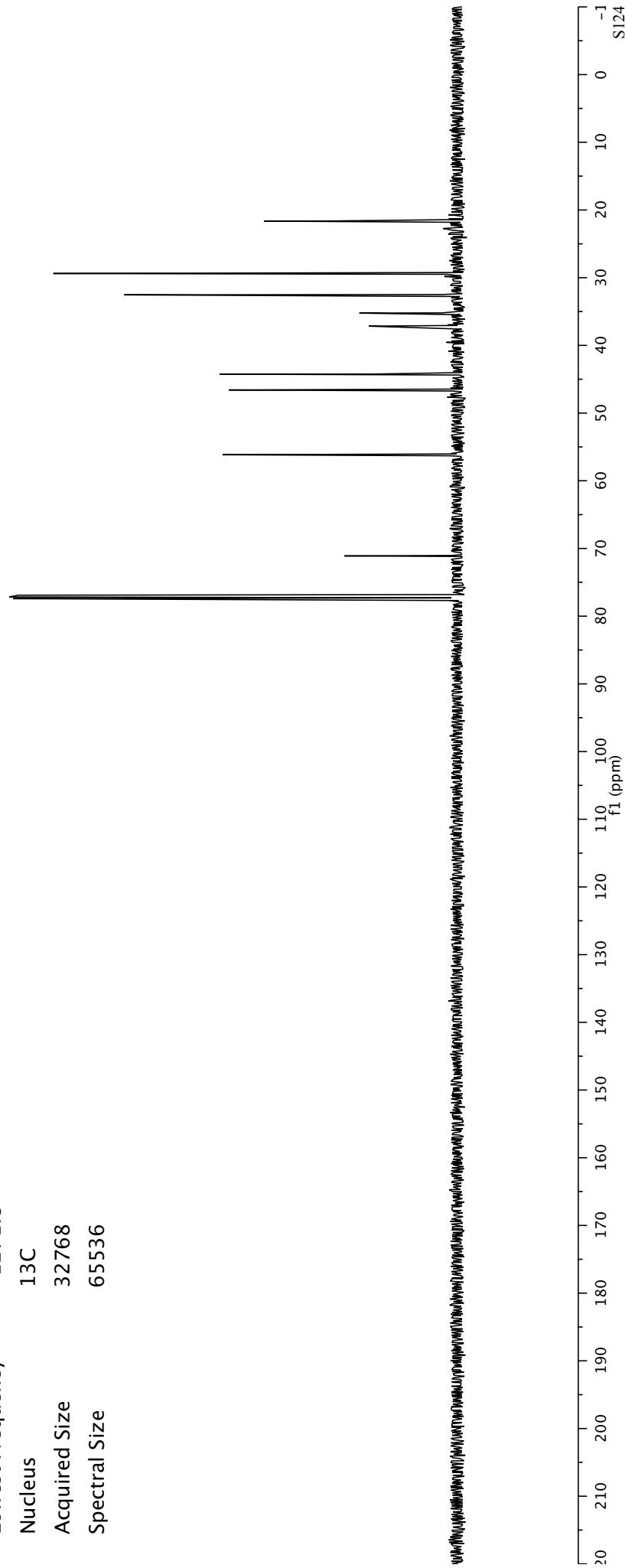
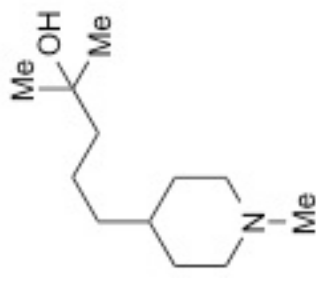
2.00 H

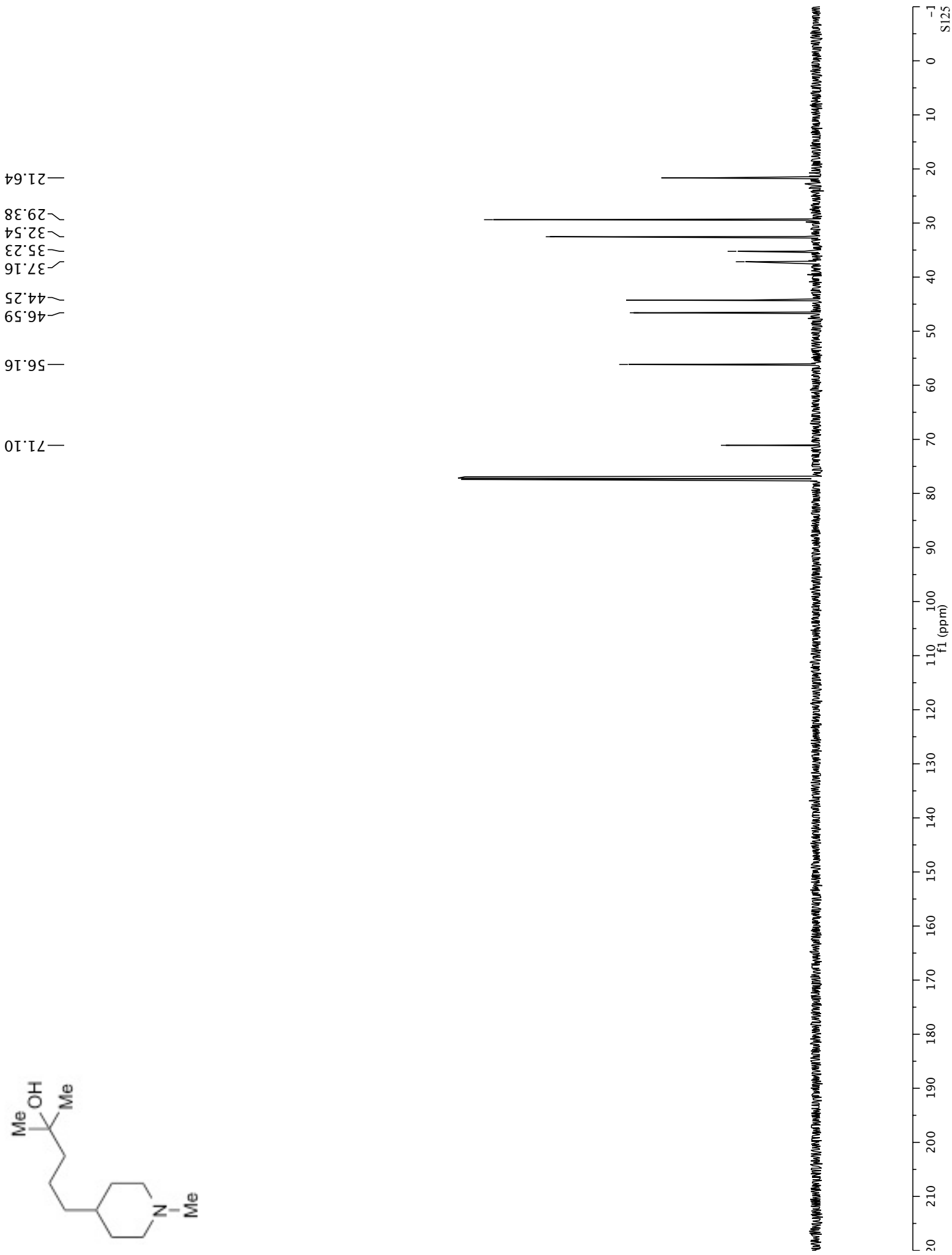
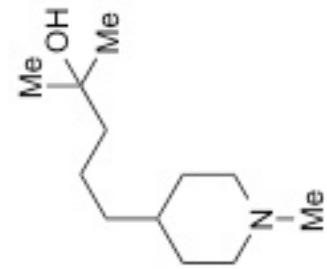
2.34
2.16
2.09
2.28
5.48
11.55
6.21

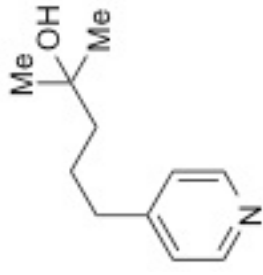
S123

f1 (ppm)

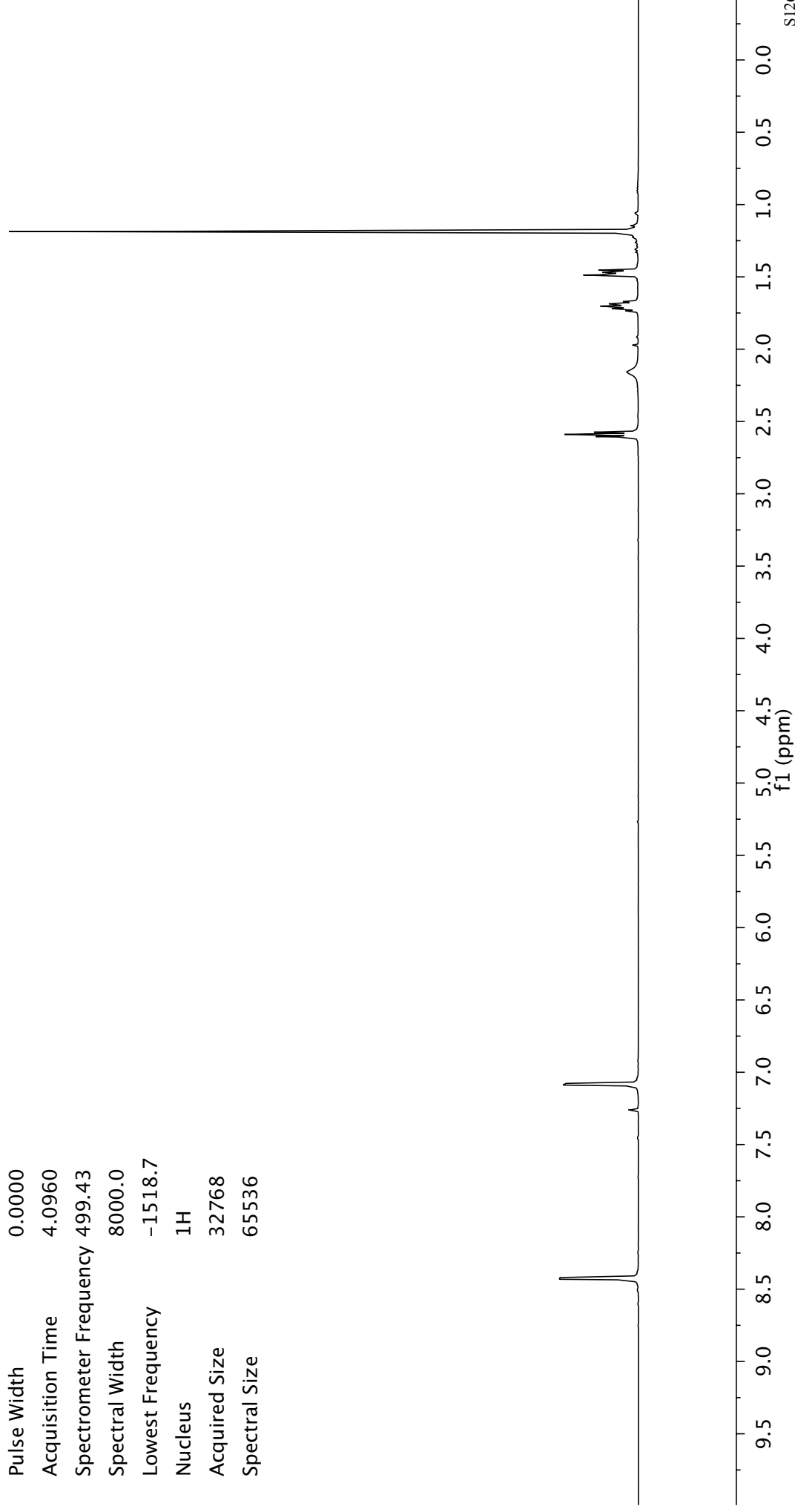
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	512
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1271.8
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

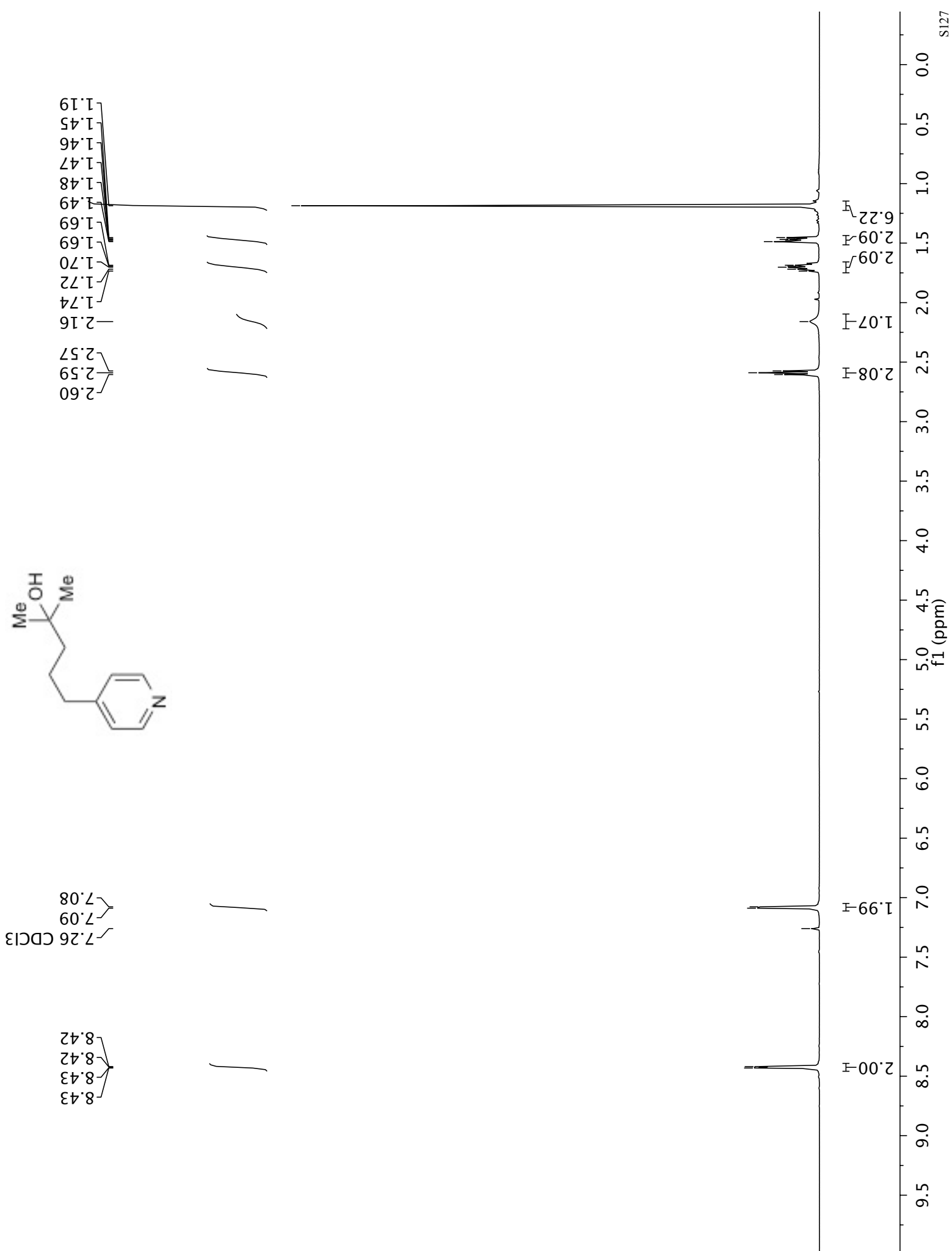


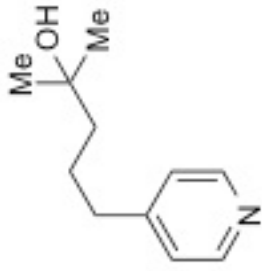




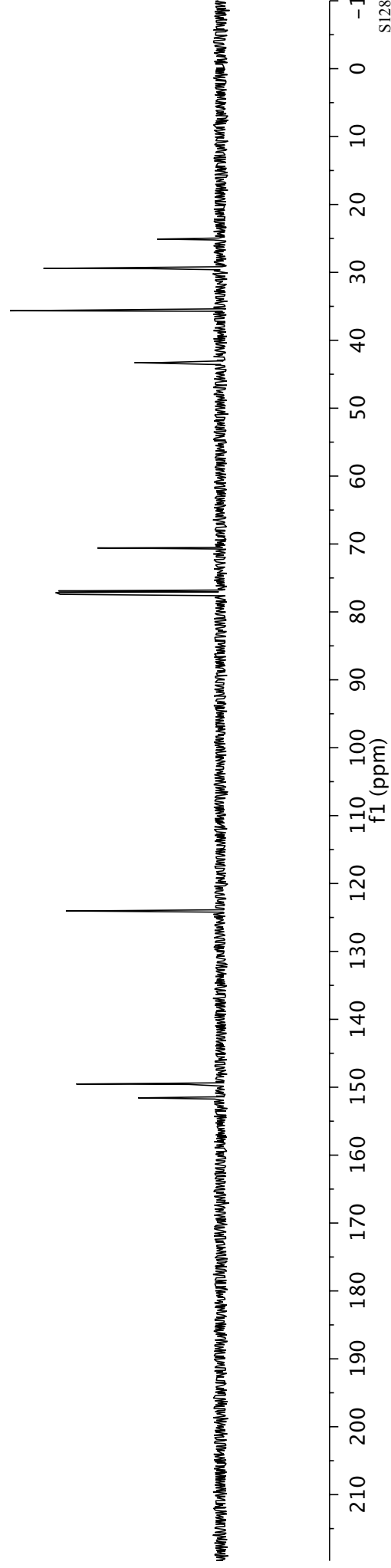
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	50
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	499.43
Spectral Width	8000.0
Lowest Frequency	-1518.7
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

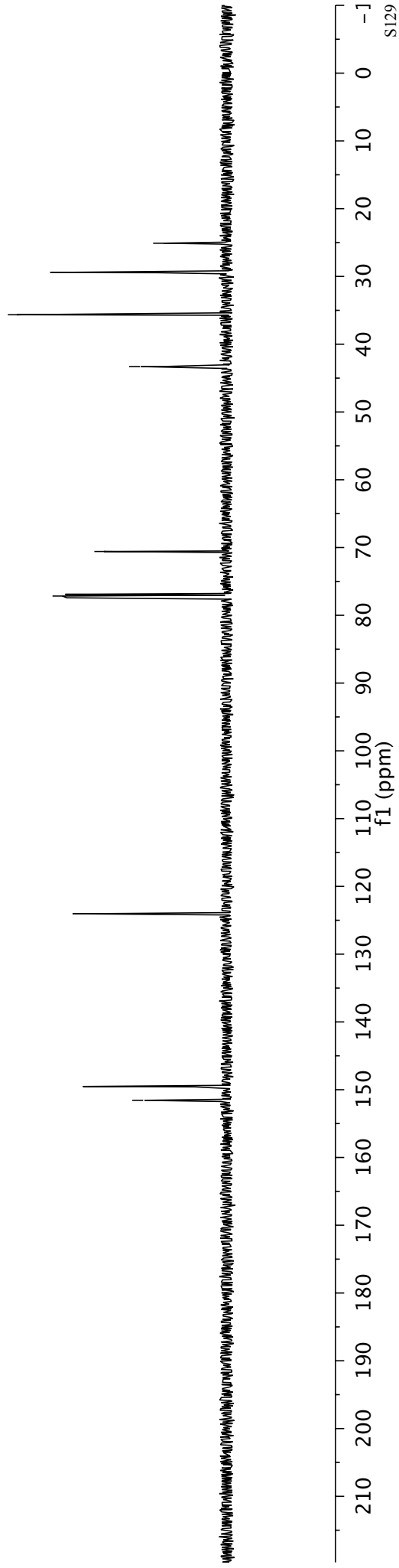
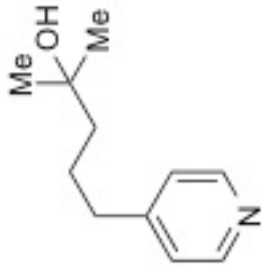


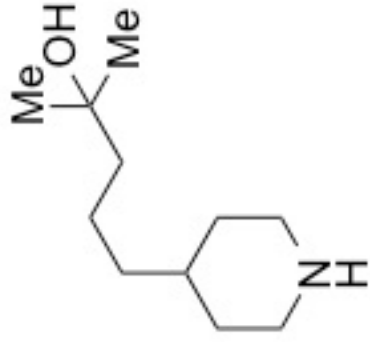




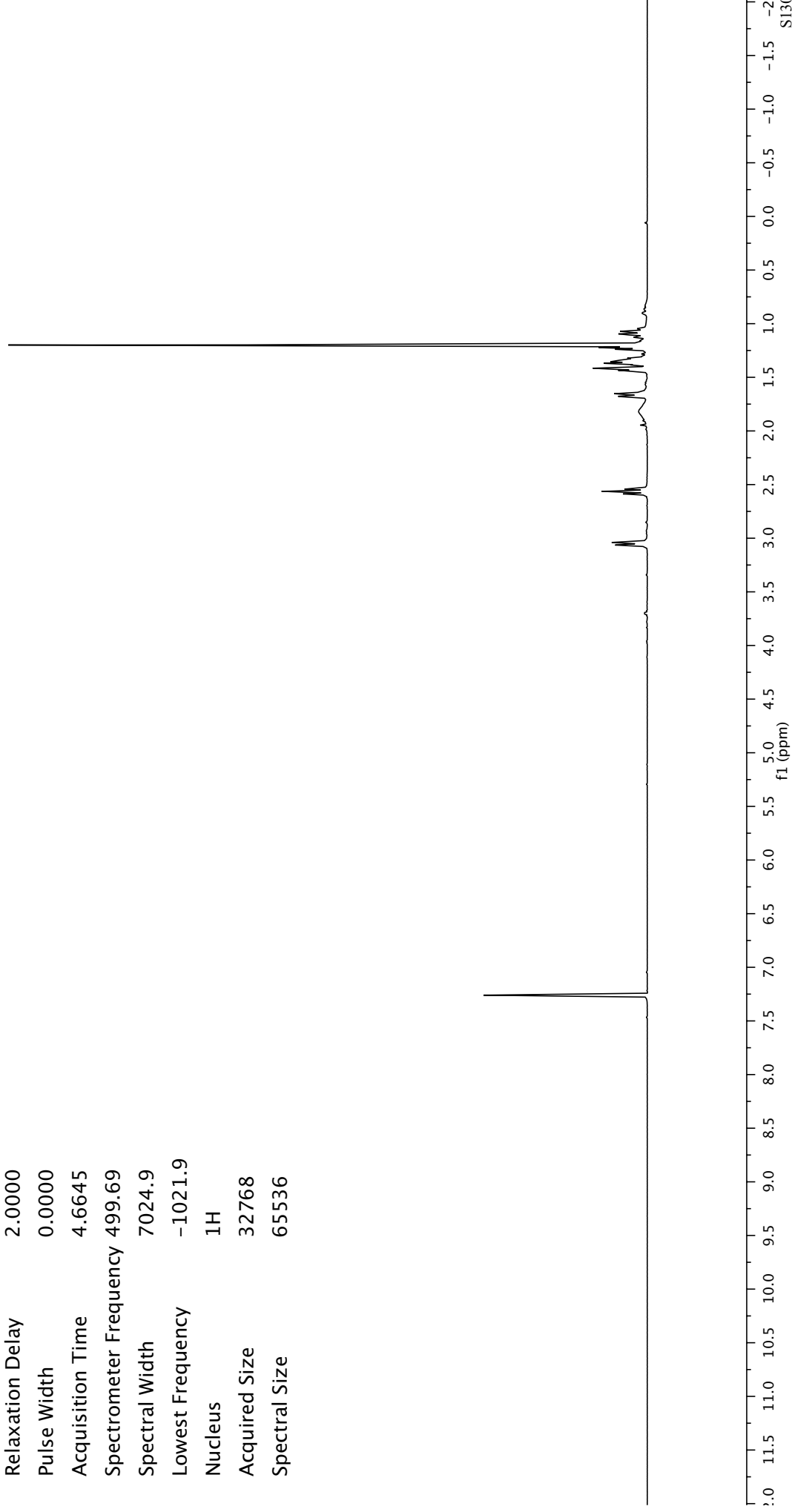
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2208.6
Nucleus	¹³ C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

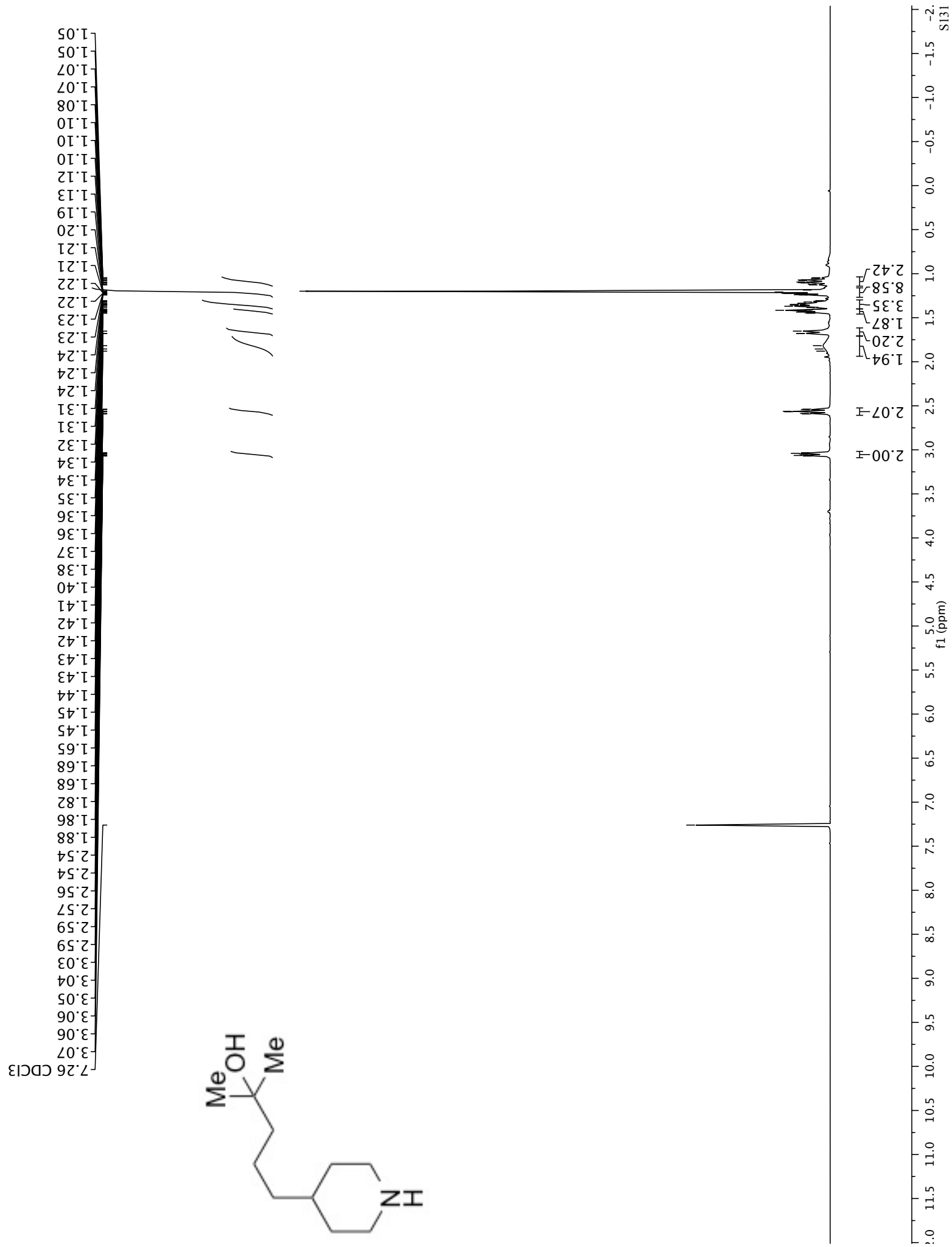
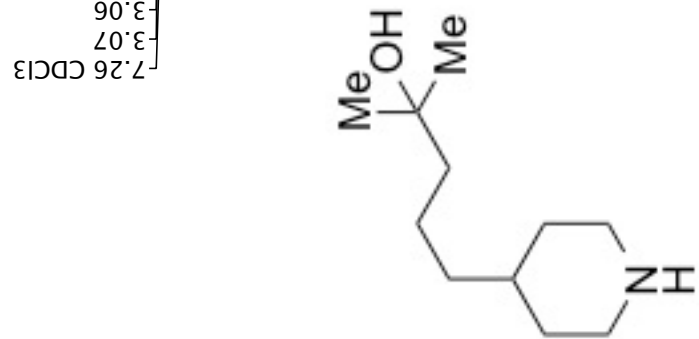






Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	16
Receiver Gain	46
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.69
Spectral Width	7024.9
Lowest Frequency	-1021.9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

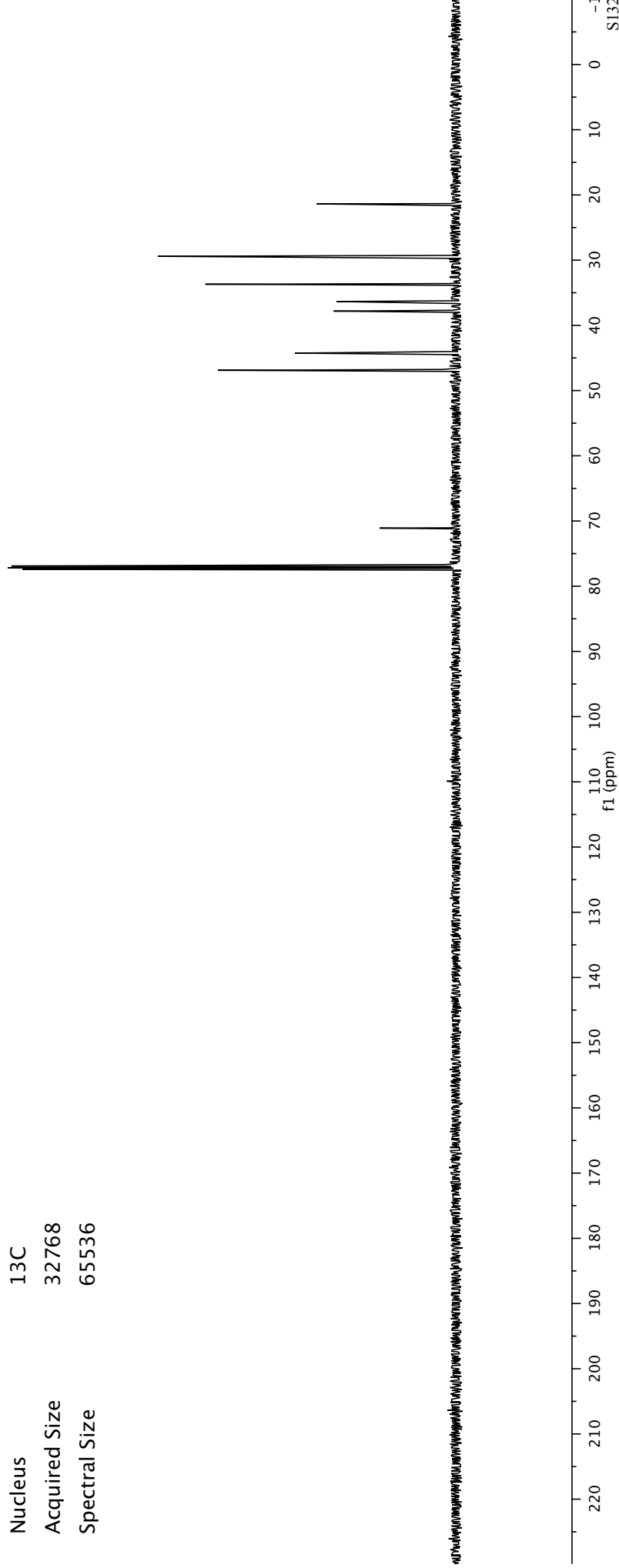
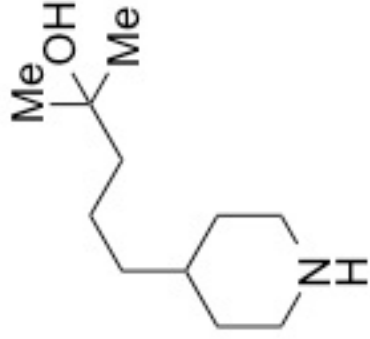


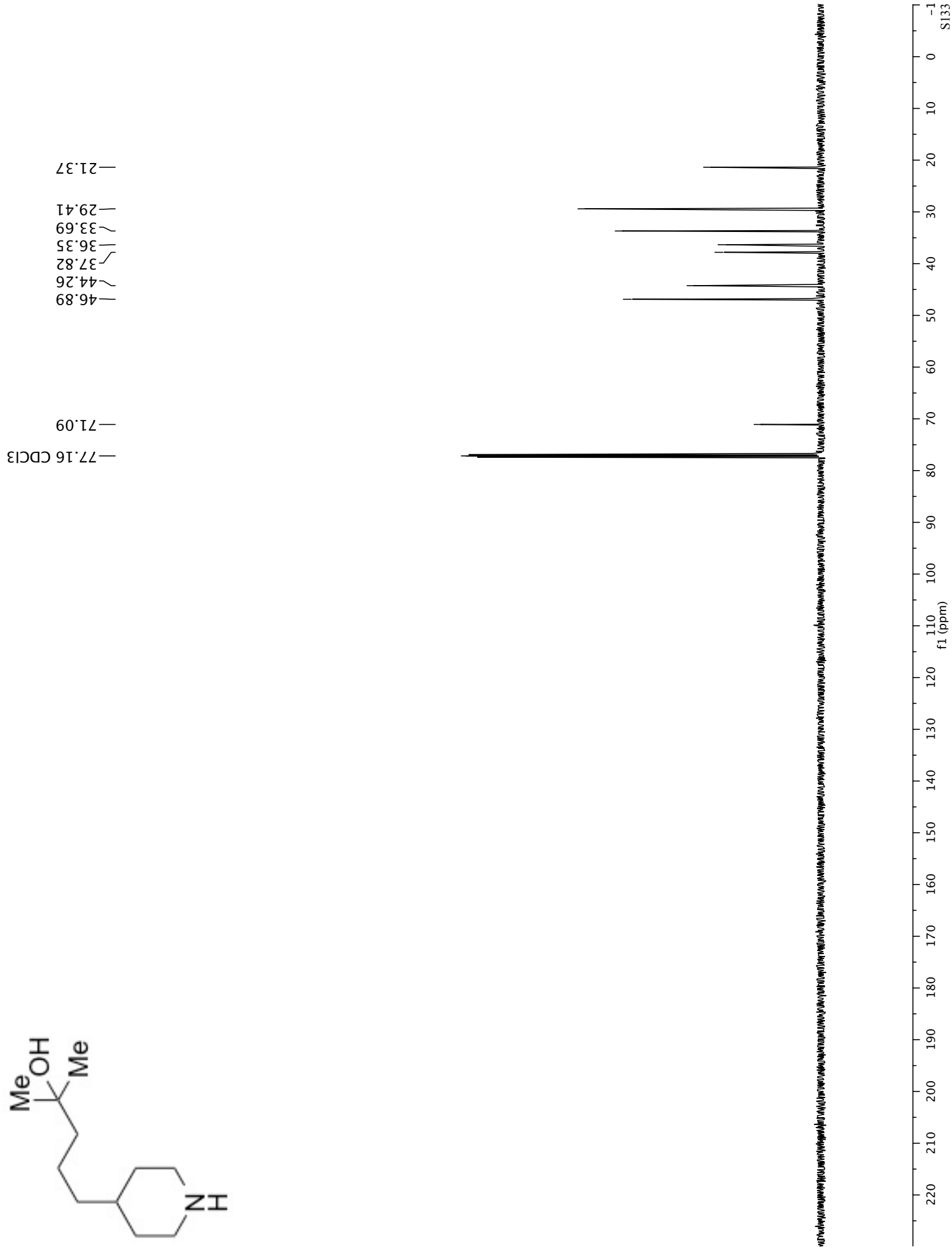
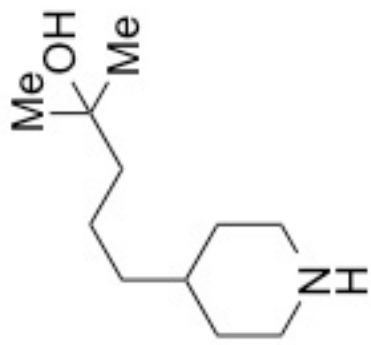


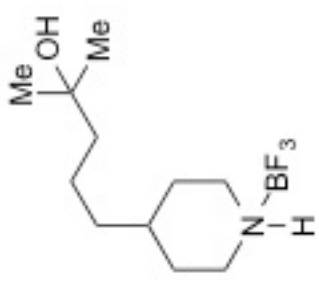
Parameter

Value

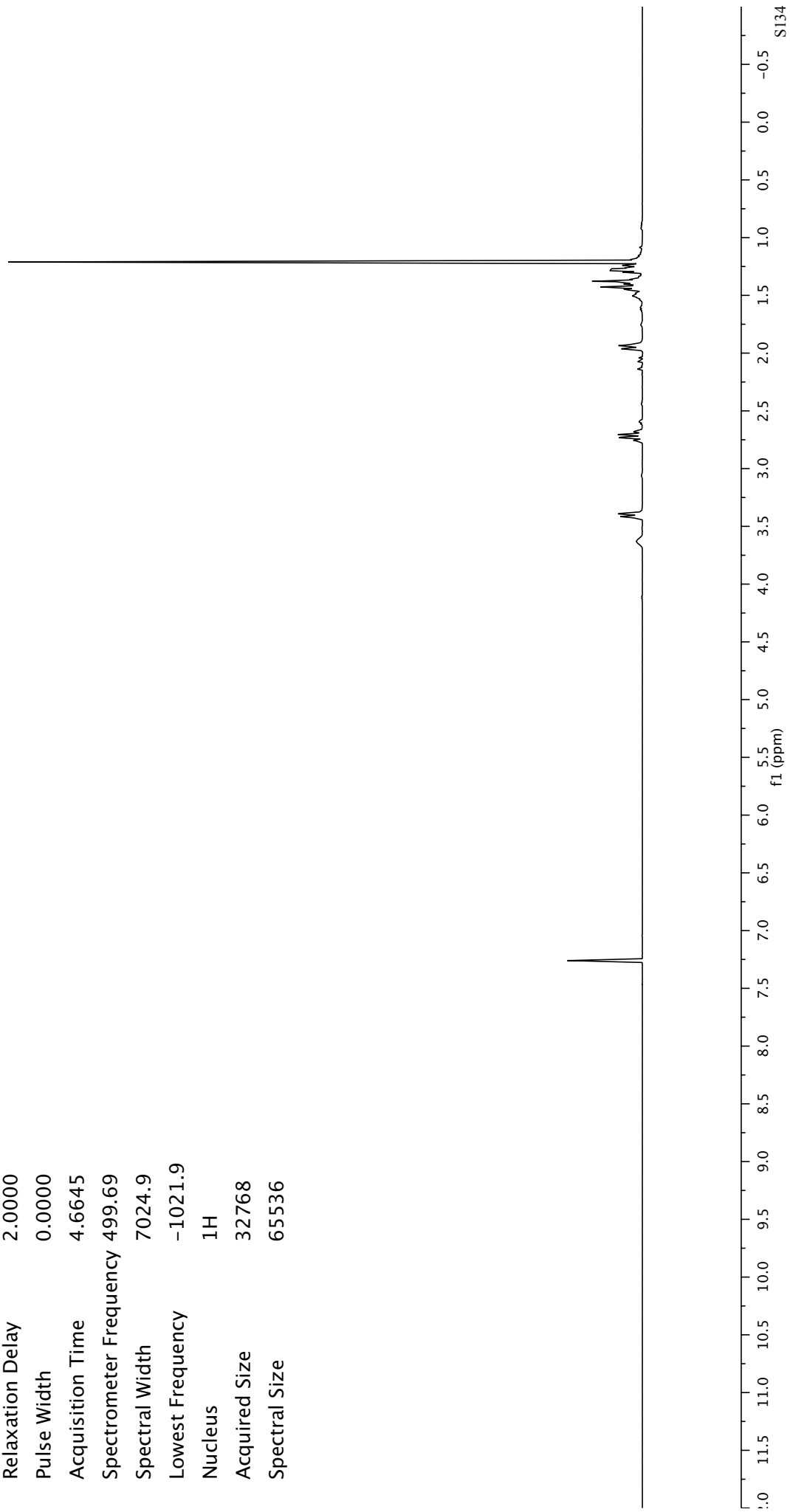
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	611
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1273.1
Nucleus	13C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

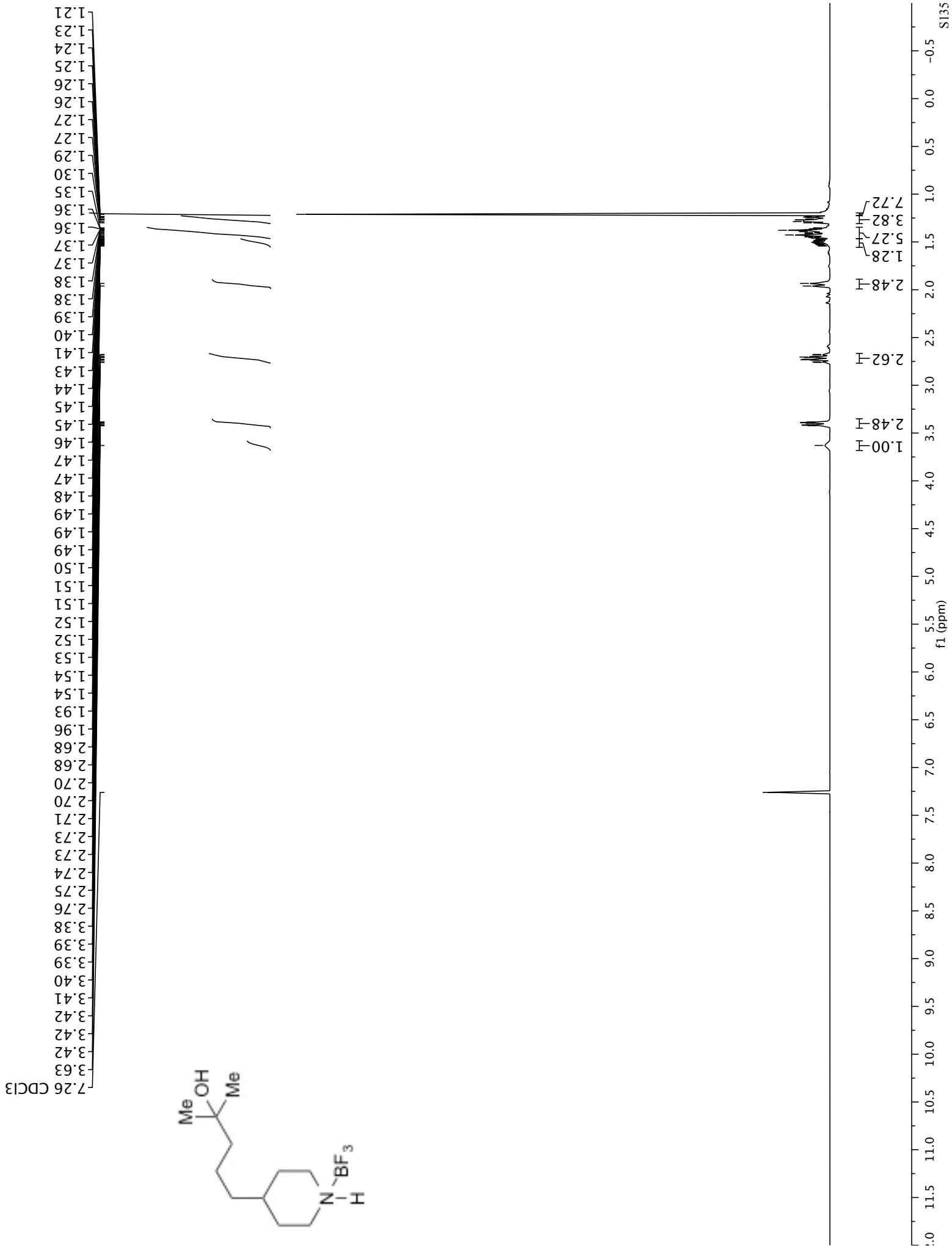
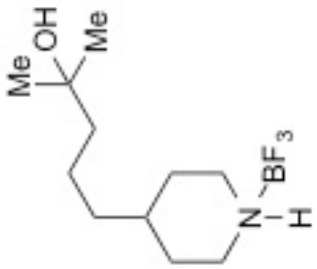




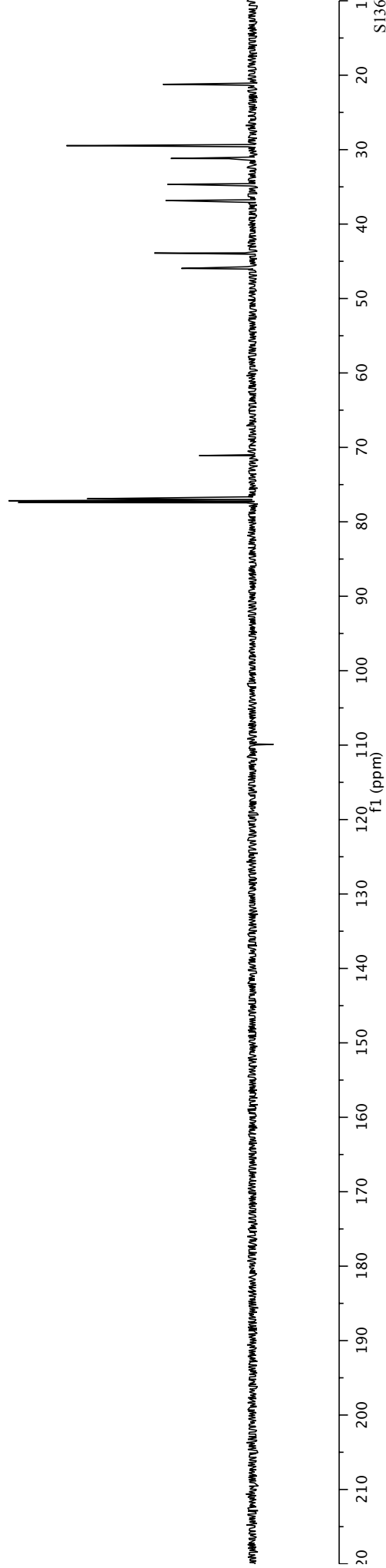
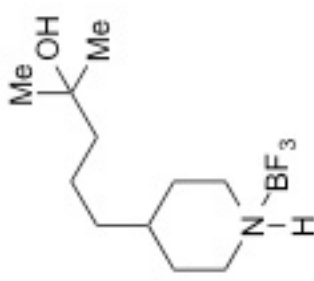


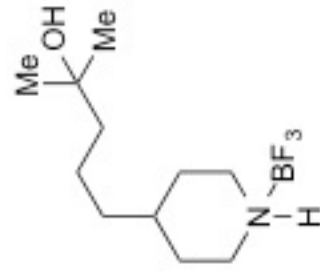
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	16
Receiver Gain	48
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.69
Spectral Width	7024.9
Lowest Frequency	-1021.9
Nucleus	1H
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





— 77.16 CDCl₃

— 71.10

— 45.96

— 43.89

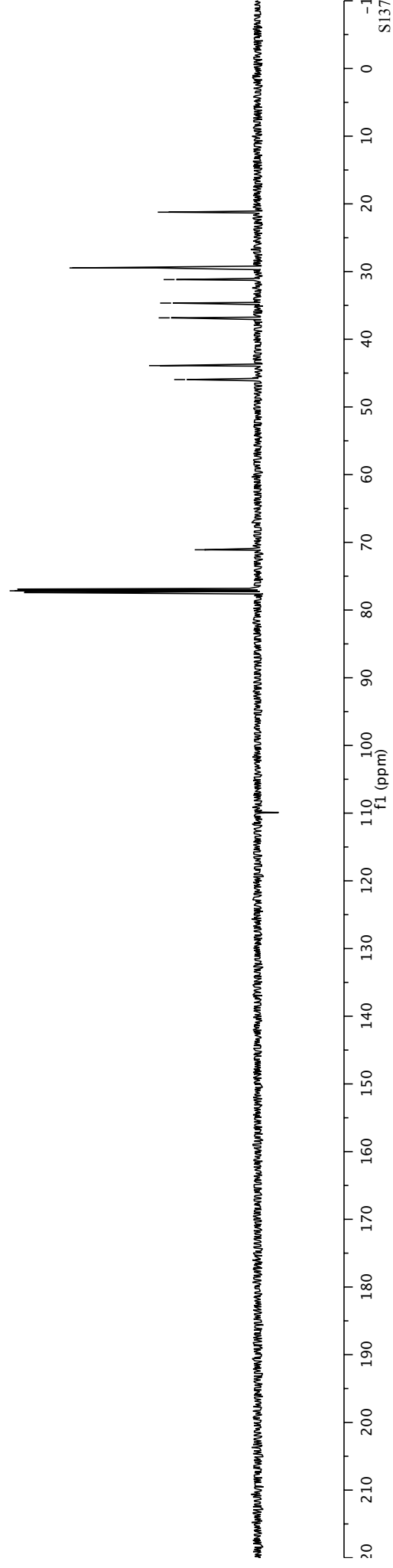
— 36.84

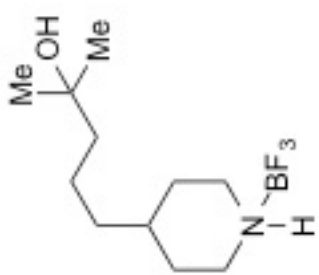
— 34.66

— 31.19

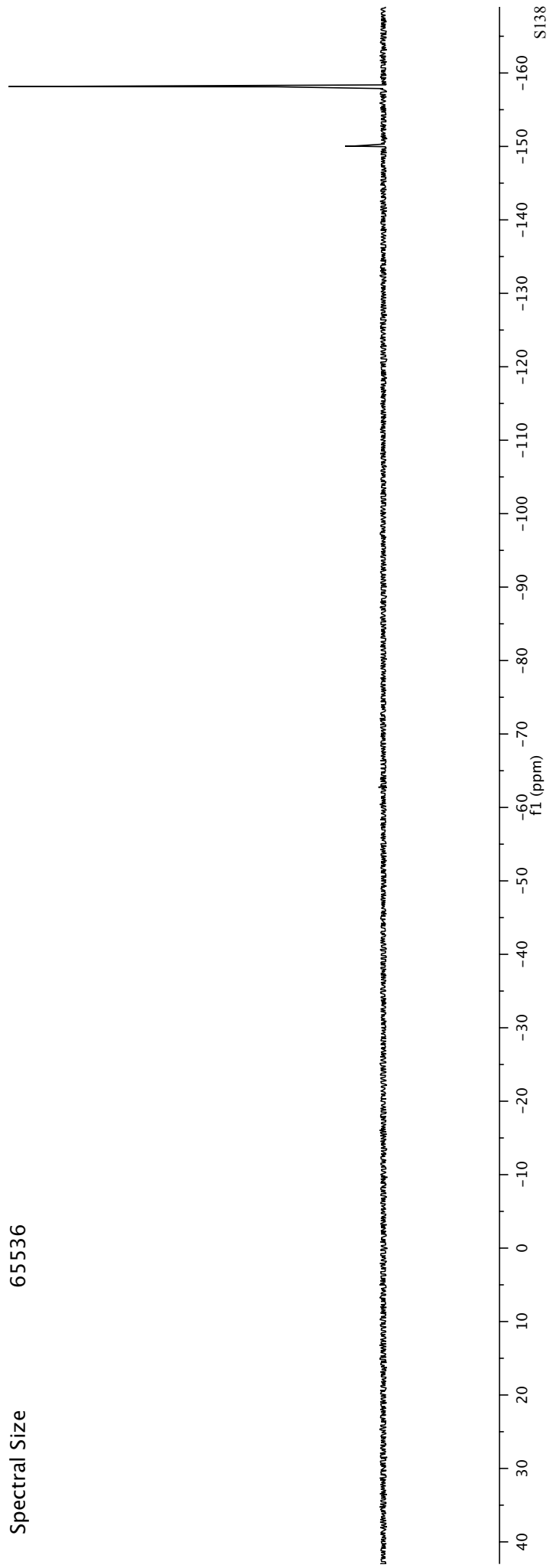
— 29.46

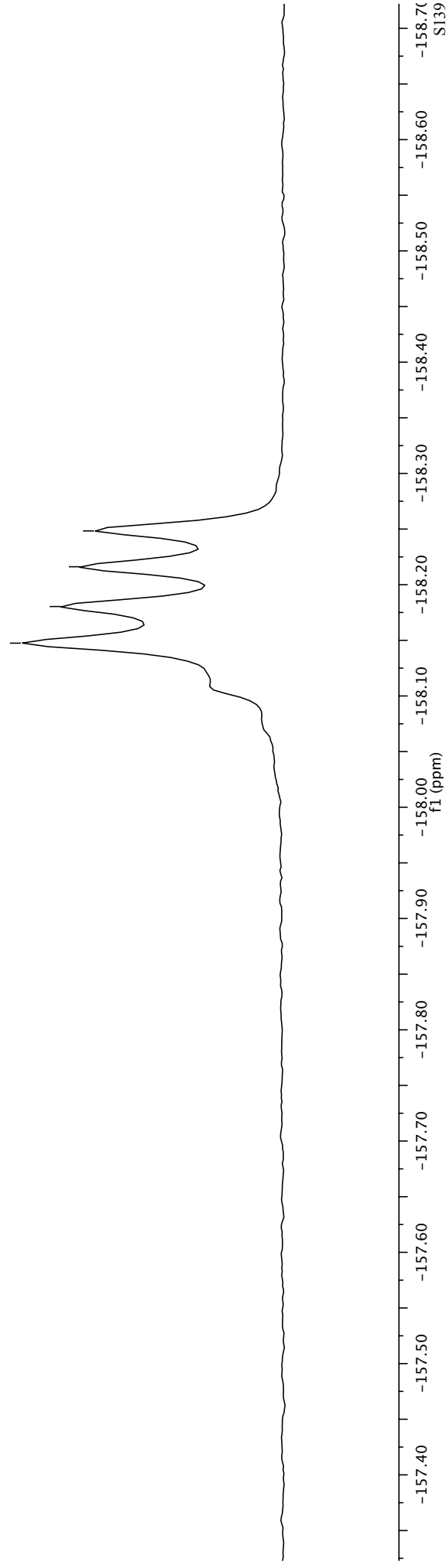
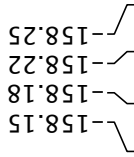
— 21.23

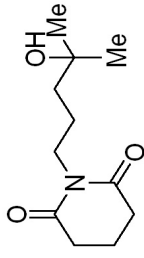




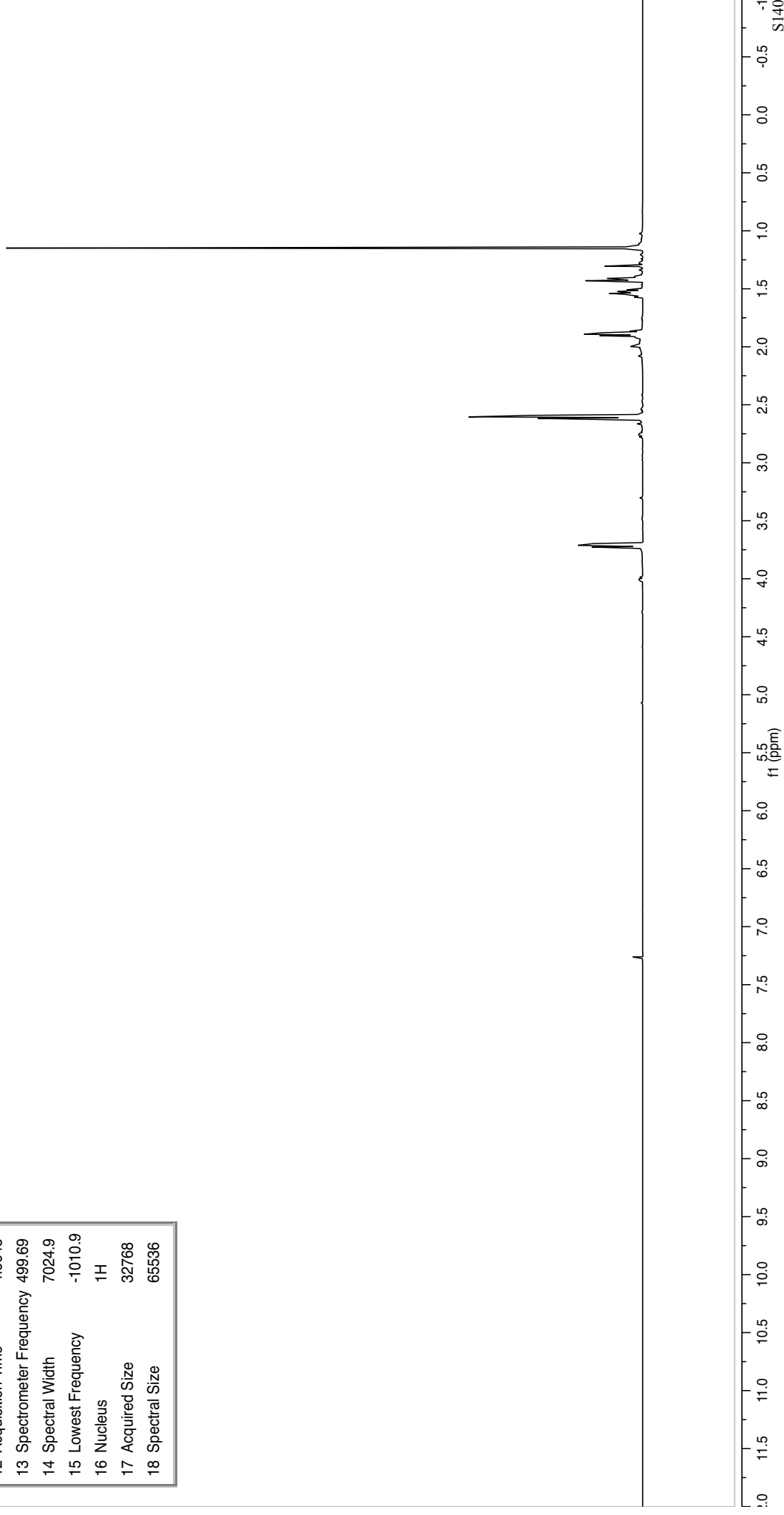
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	132
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency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

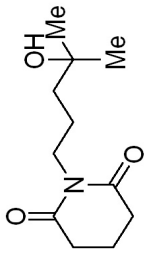




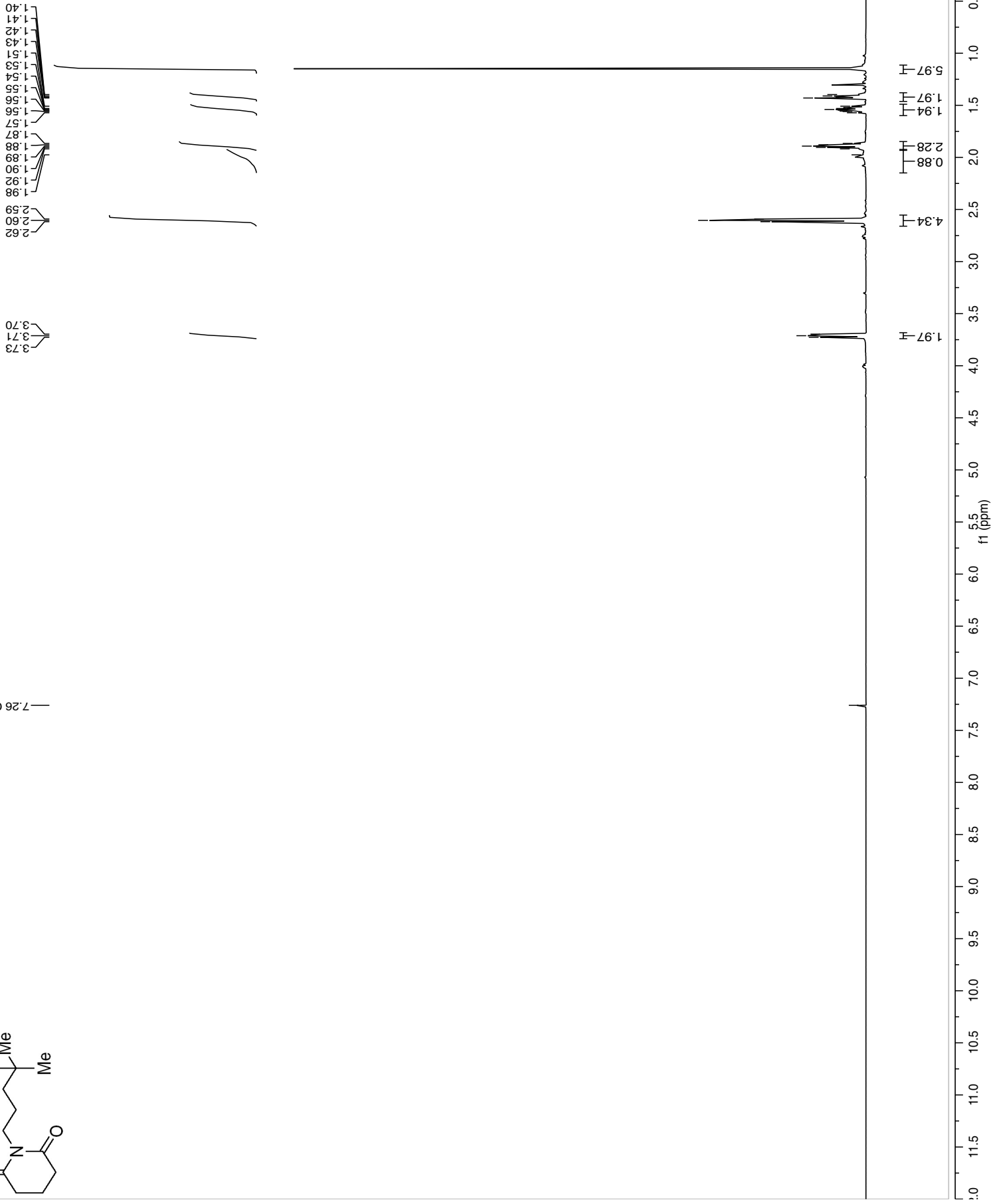


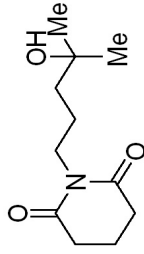
Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	8
9 Receiver Gain	36
10 Relaxation Delay	0.0000
11 Pulse Width	0.0000
12 Acquisition Time	4.6645
13 Spectrometer Frequency	499.69
14 Spectral Width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



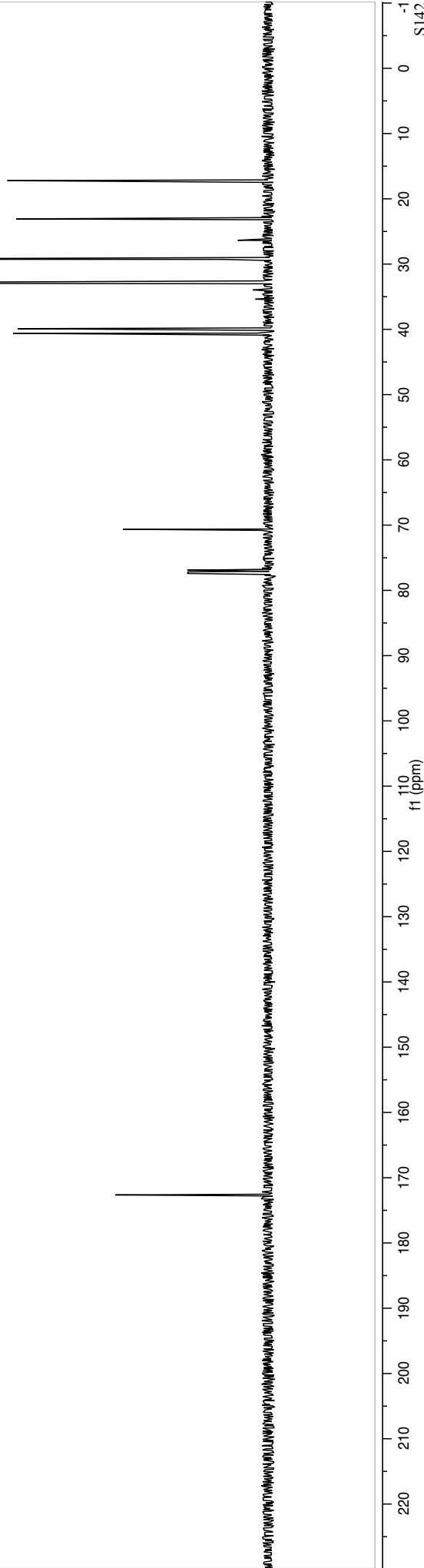


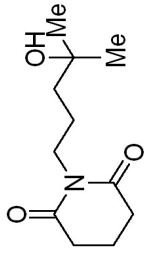
7.26 CDCl₃



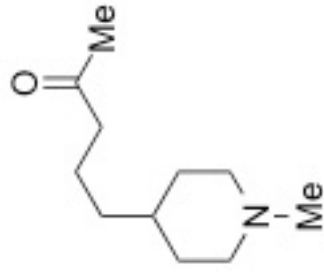


Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	48
9 Receiver Gain	60
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.0863
13 Spectrometer Frequency	125.66
14 Spectral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

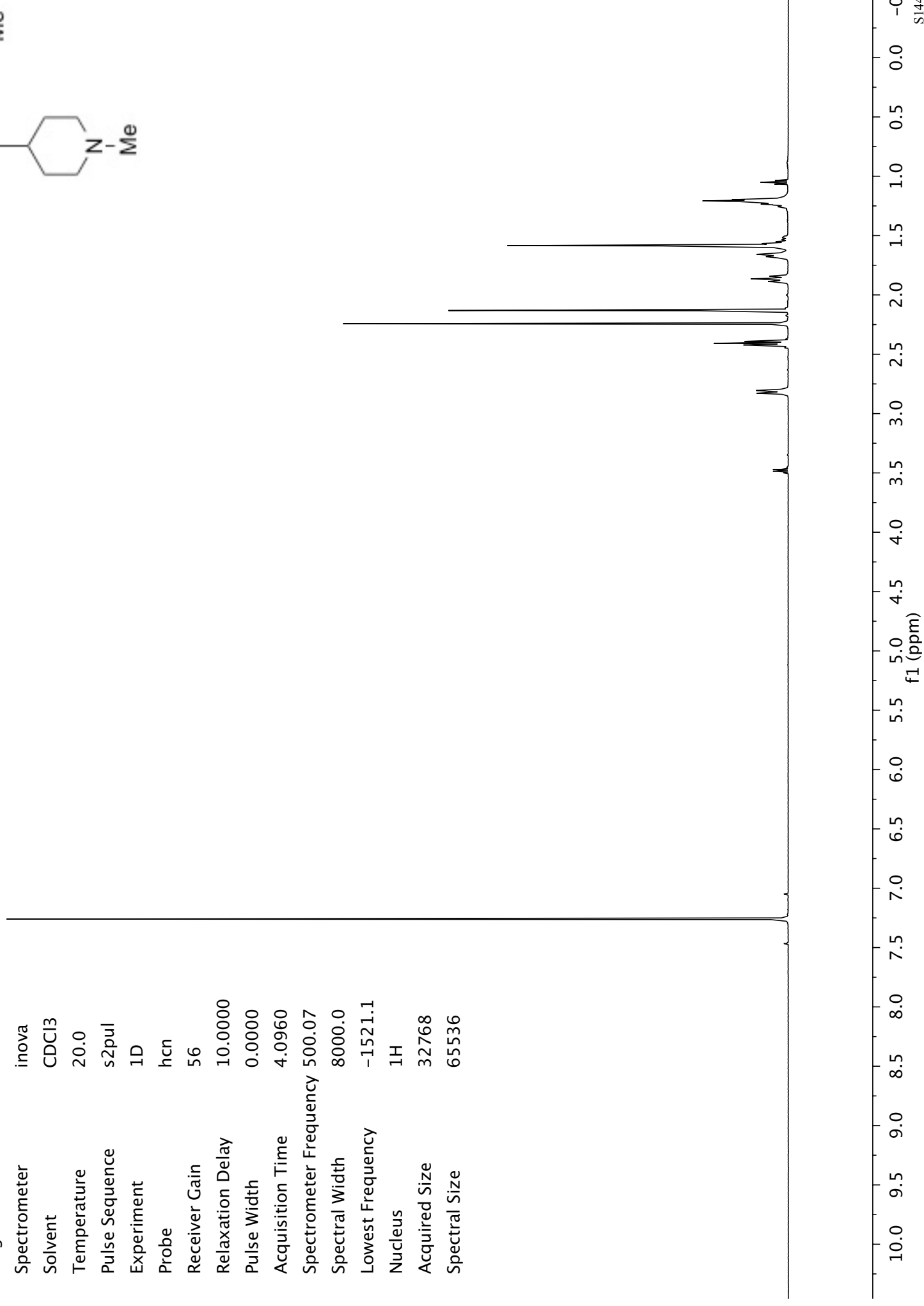


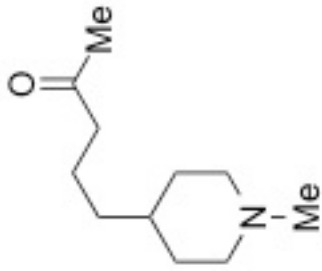


SI43
-1
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
220
f1 (ppm)

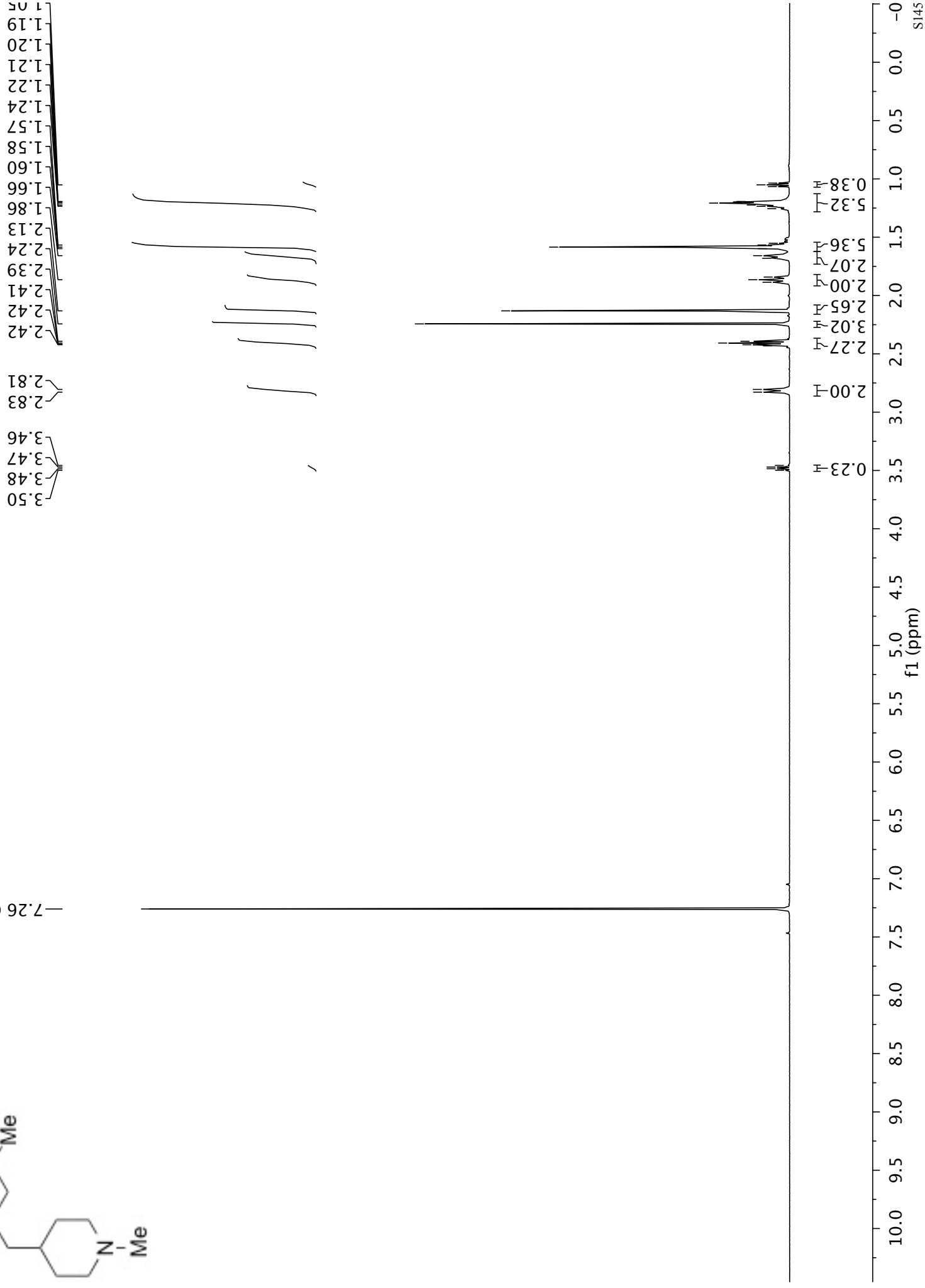


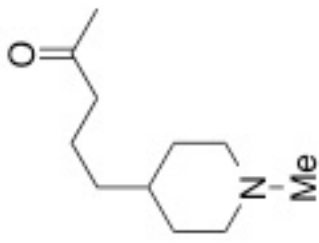
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	56
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	¹ H
Acquired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



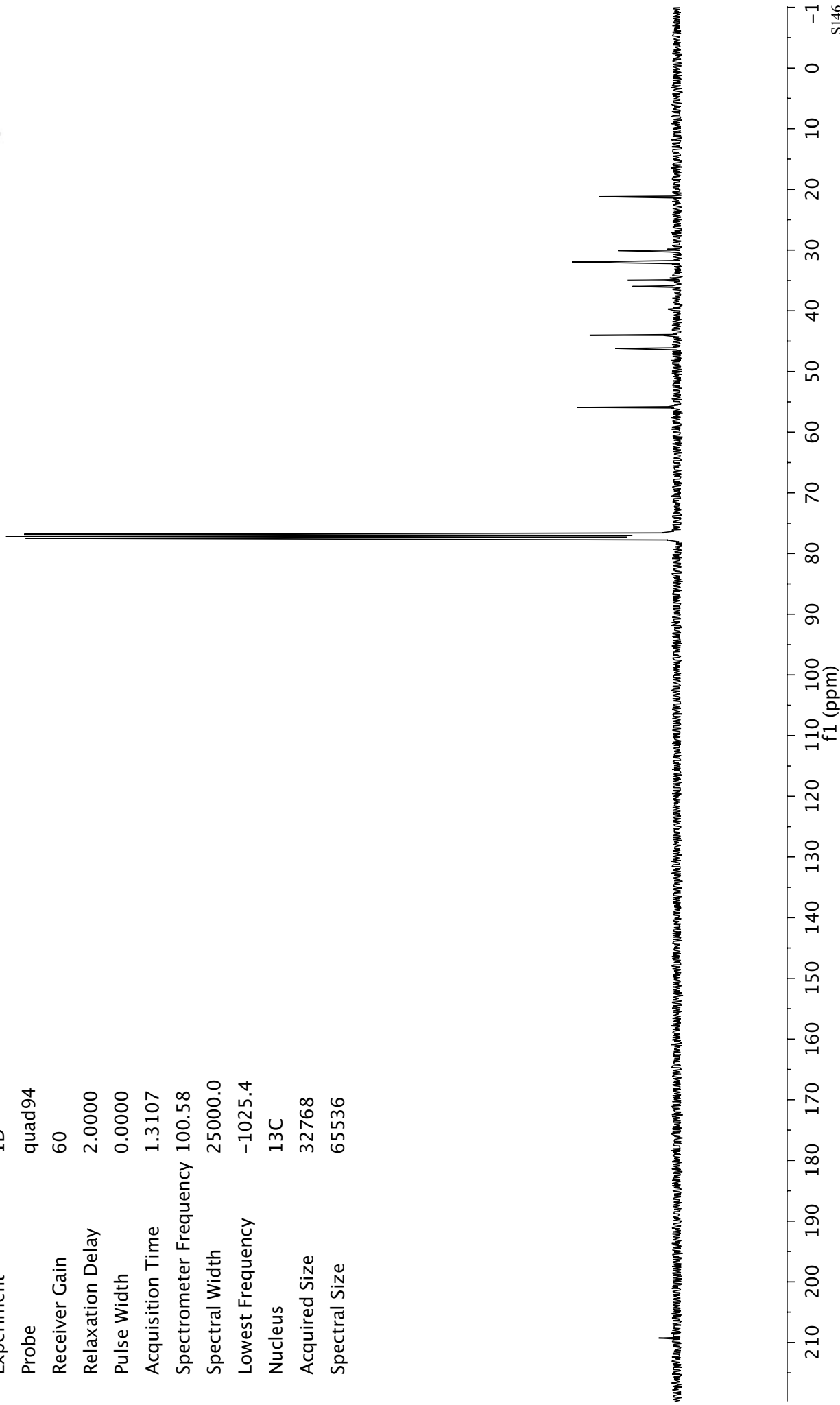


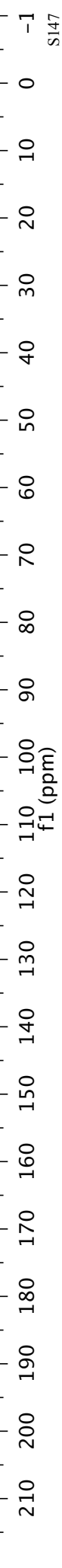
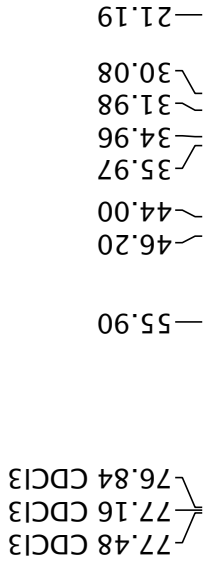
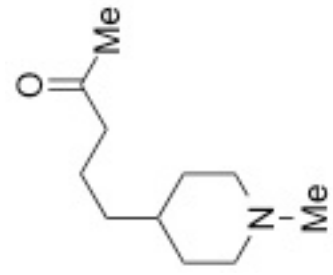
— 7.26 CDCl₃

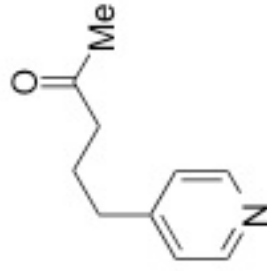




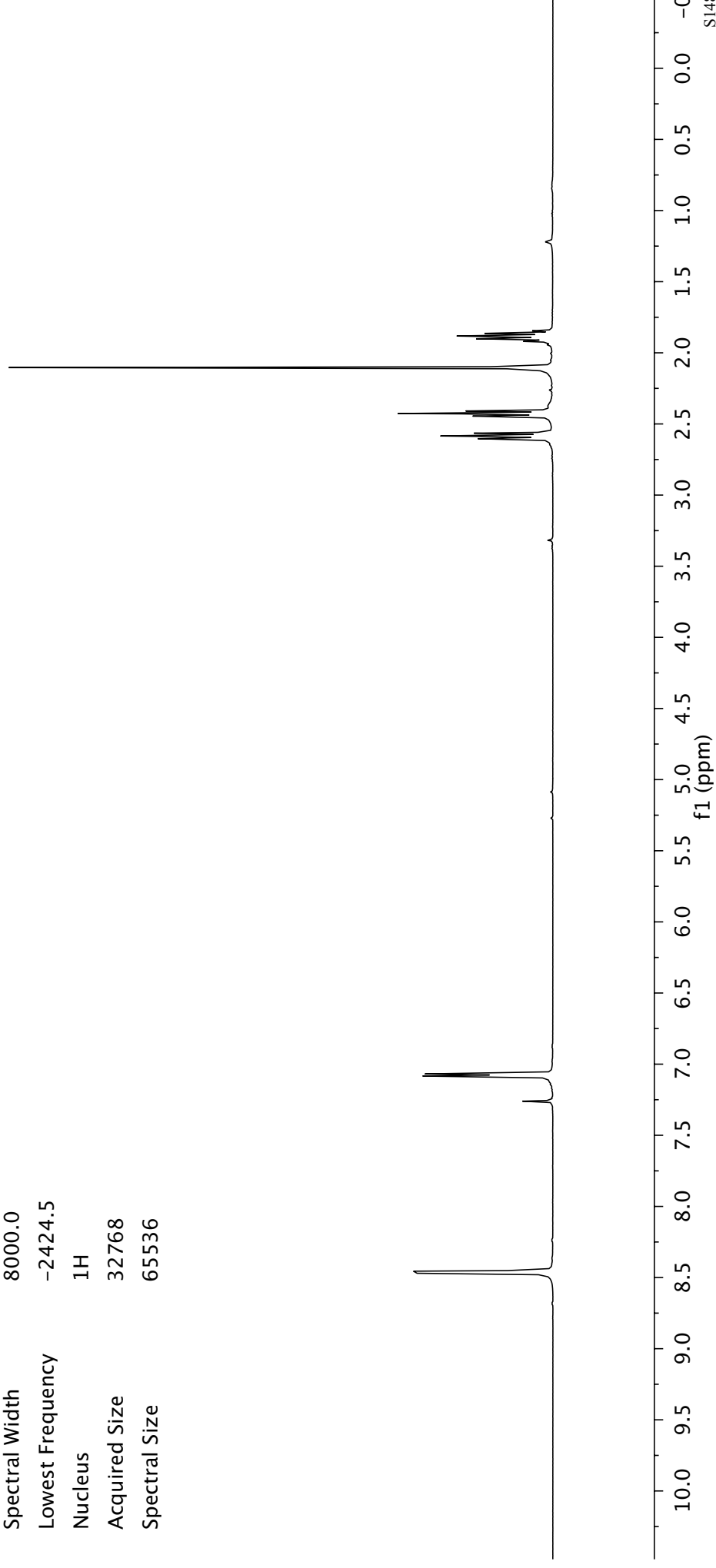
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.3107
Spectrometer Frequency	100.58
Spectral Width	25000.0
Lowest Frequency	-1025.4
Nucleus	¹³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

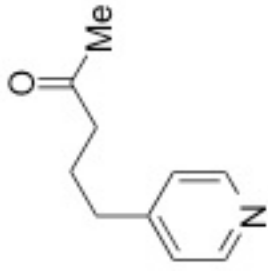






Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	46
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	399.95
Spectral Width	8000.0
Lowest Frequency	-2424.5
Nucleus	1H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





7.26 CDCl₃
7.08
7.07

8.47
8.47
8.46
8.46

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

1.97

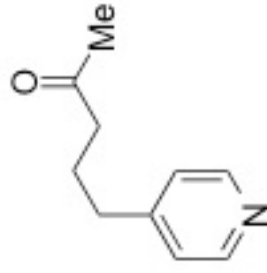
1.95

2.00
2.03
2.92
1.99

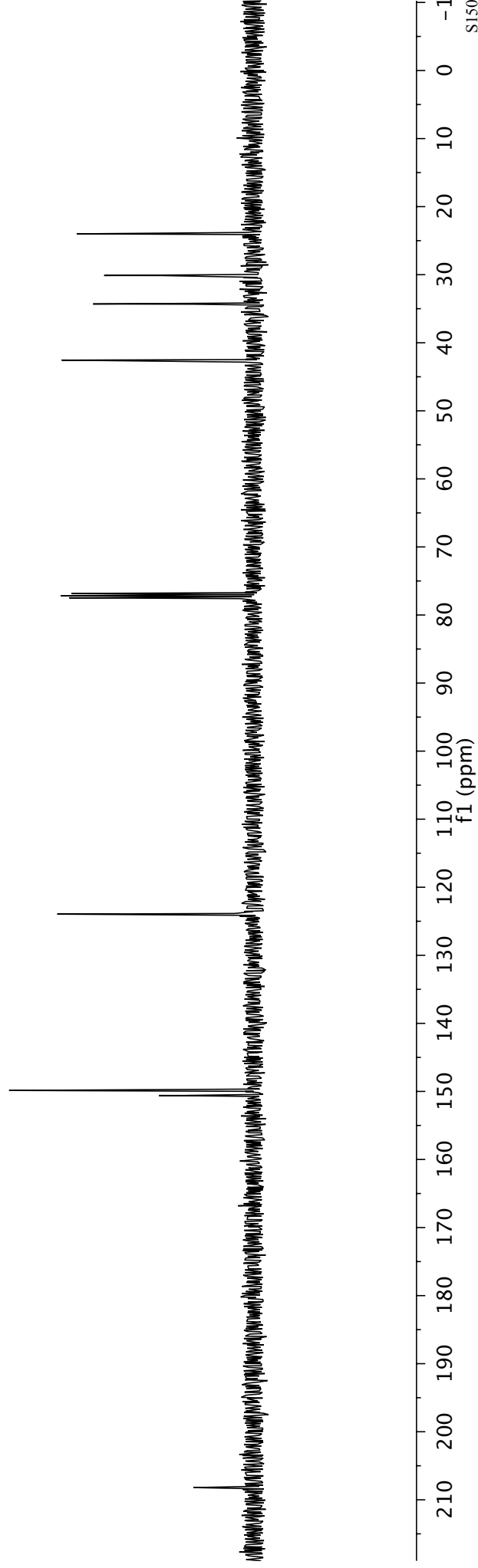
f1 (ppm)

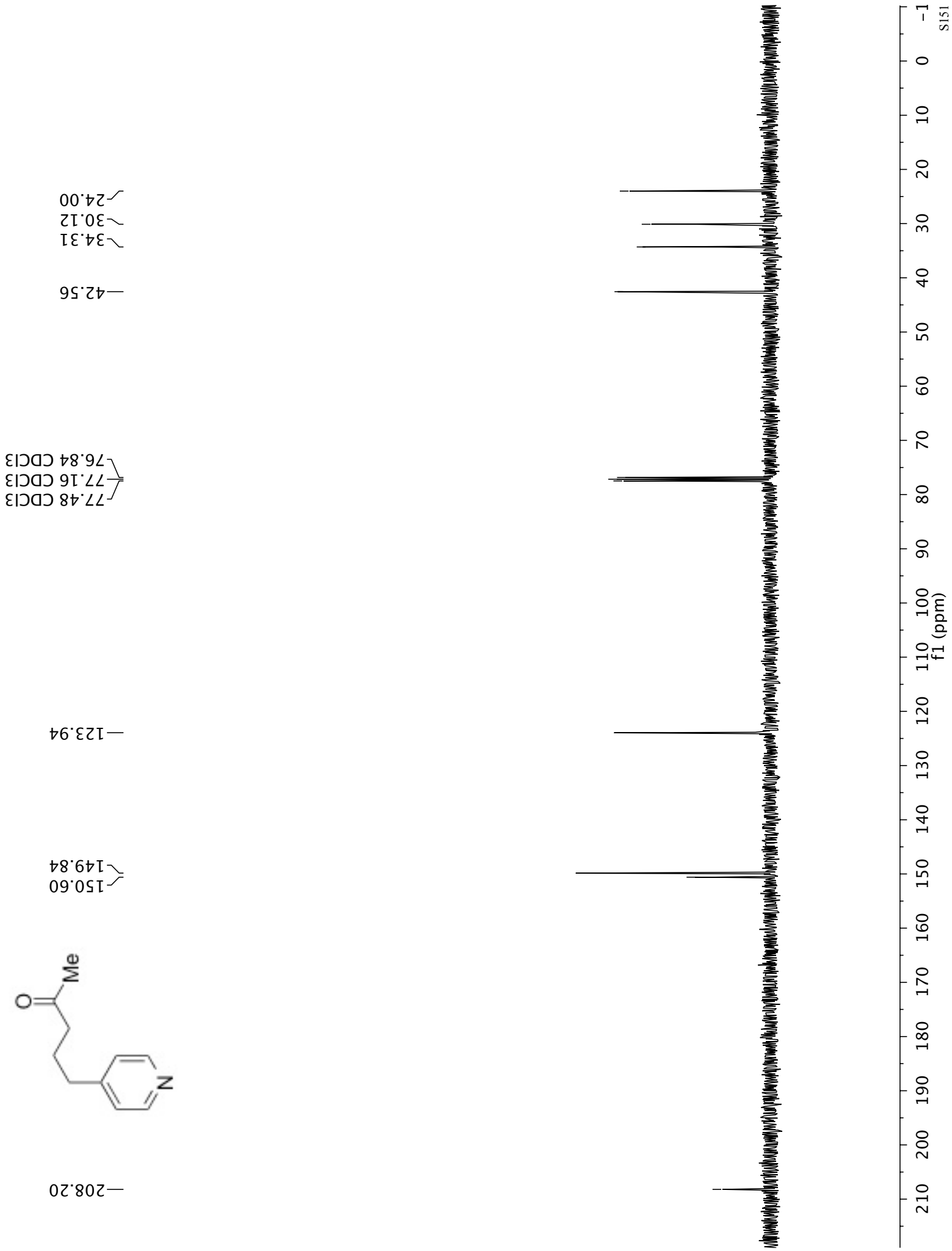
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0

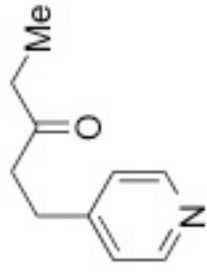
S149



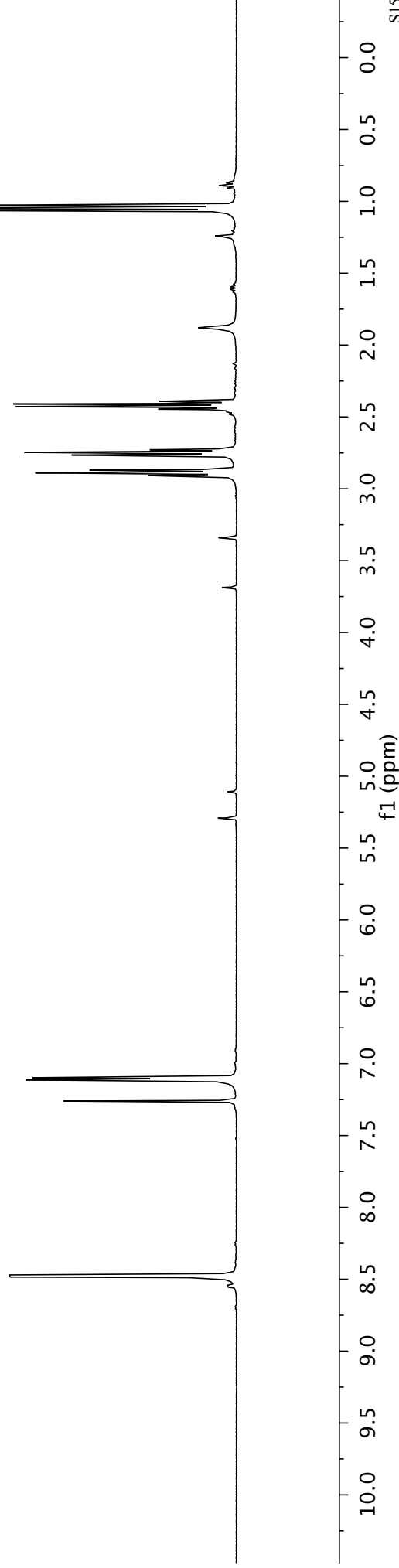
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.3107
Spectrometer Frequency	100.58
Spectral Width	25000.0
Lowest Frequency	-1031.7
Nucleus	¹³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

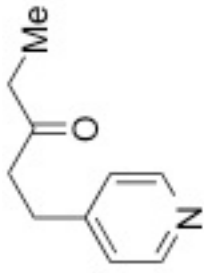






Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	58
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	399.95
Spectral Width	8000.0
Lowest Frequency	-2424.5
Nucleus	1H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





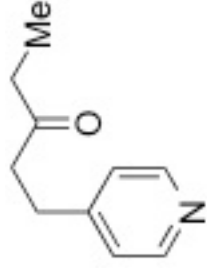
8.49
8.48
8.47
8.47
7.26 CDCl₃
7.11
7.10

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

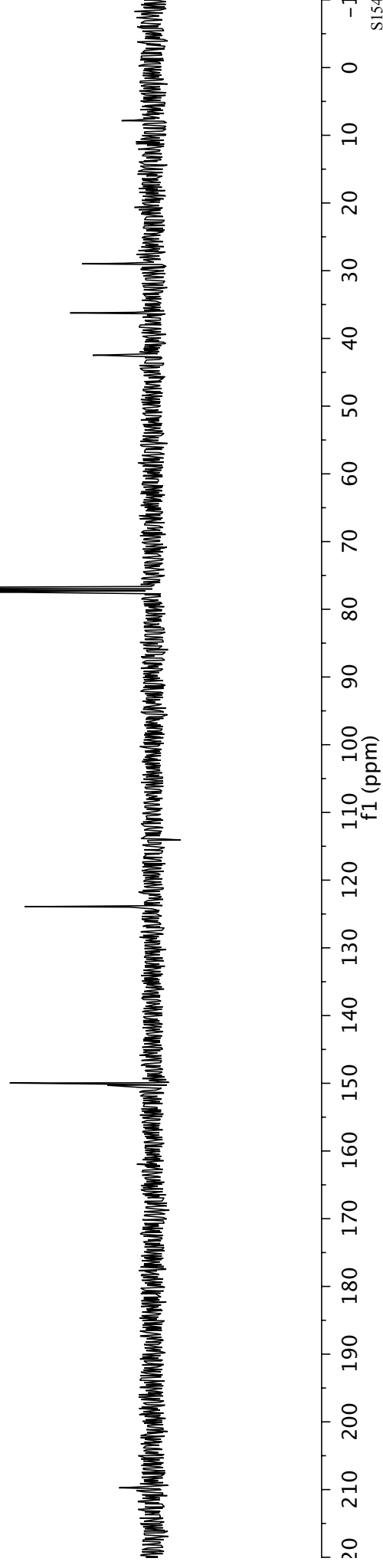
1.87
1.98
2.00
2.01
2.05
2.96

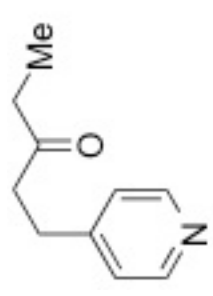
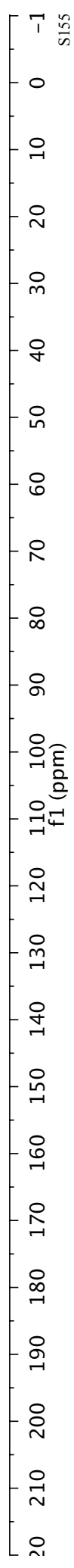
f1 (ppm)

S153



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	-1026.6
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536





—209.74

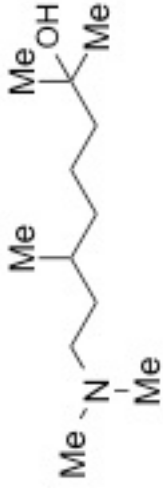
150.30
149.96

—123.92

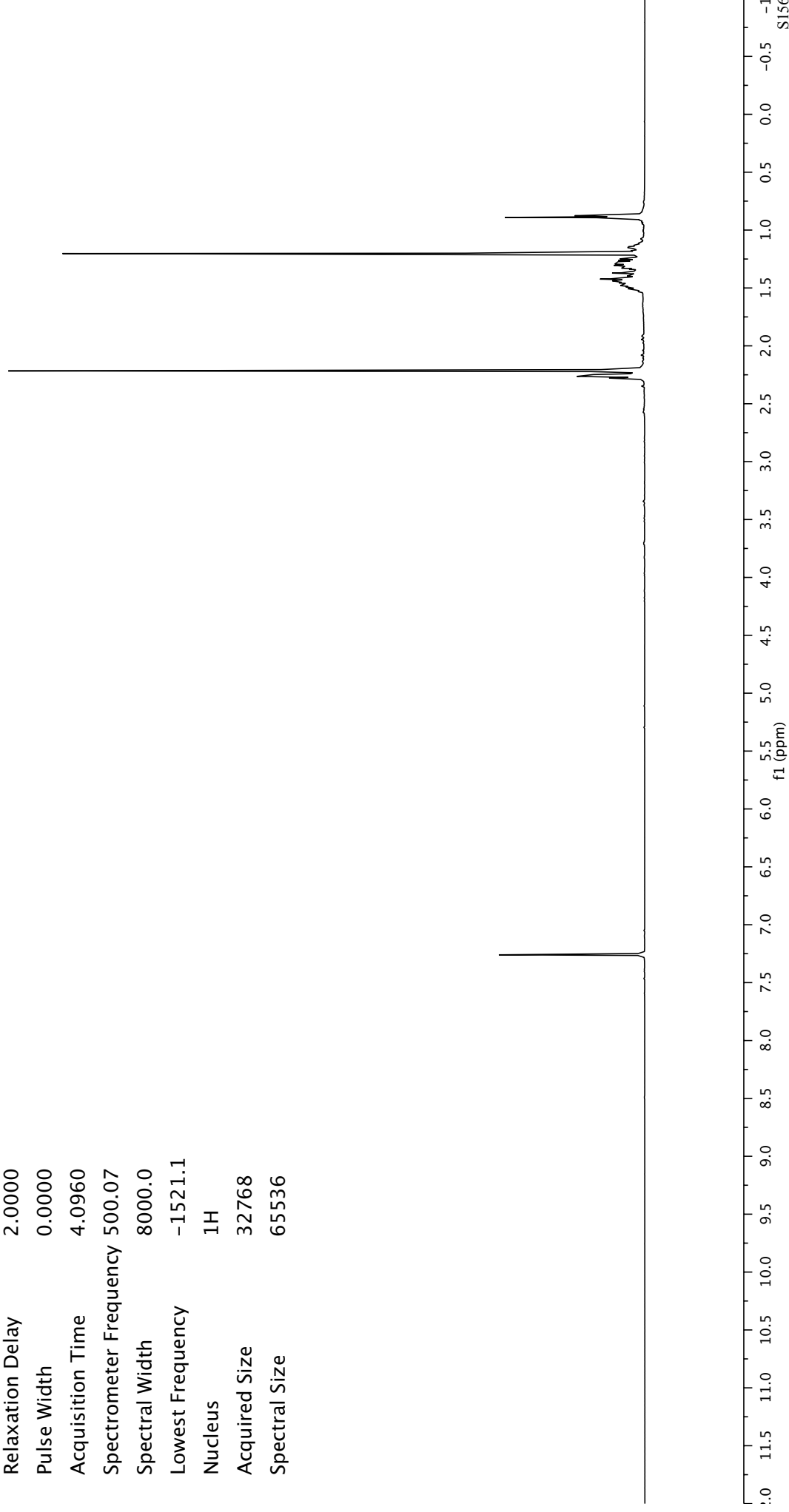
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3

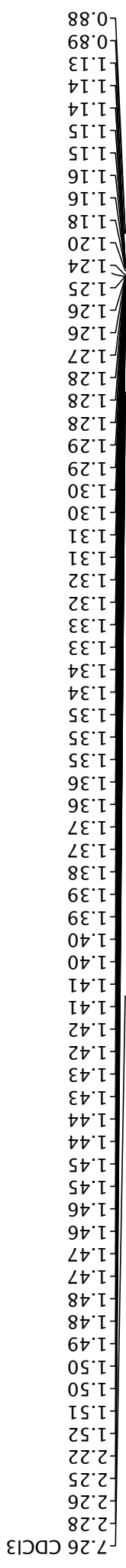
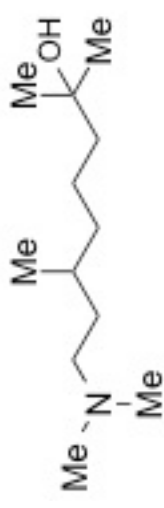
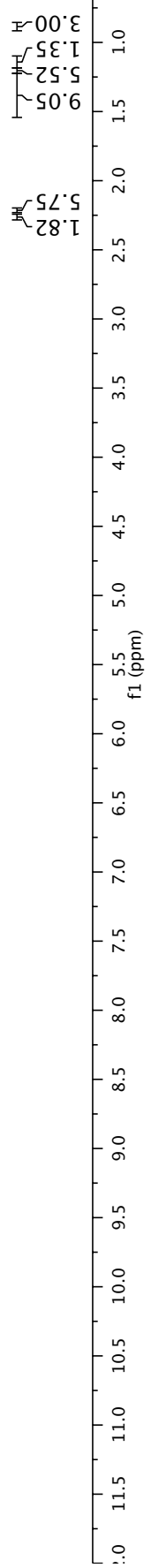
42.47
36.24
28.98

—7.84

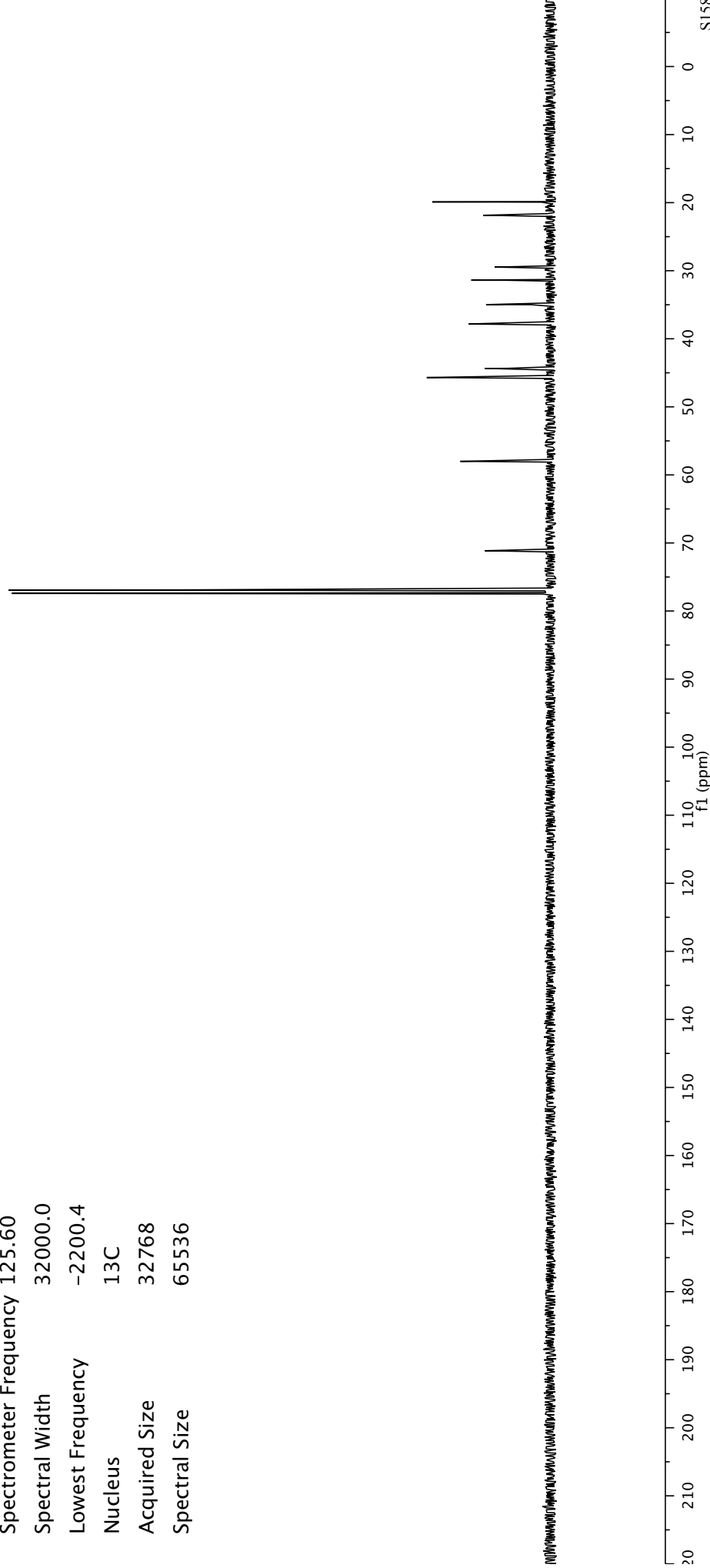
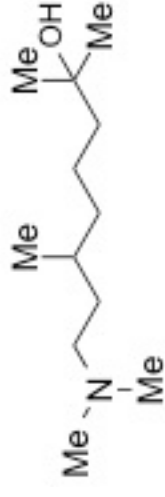


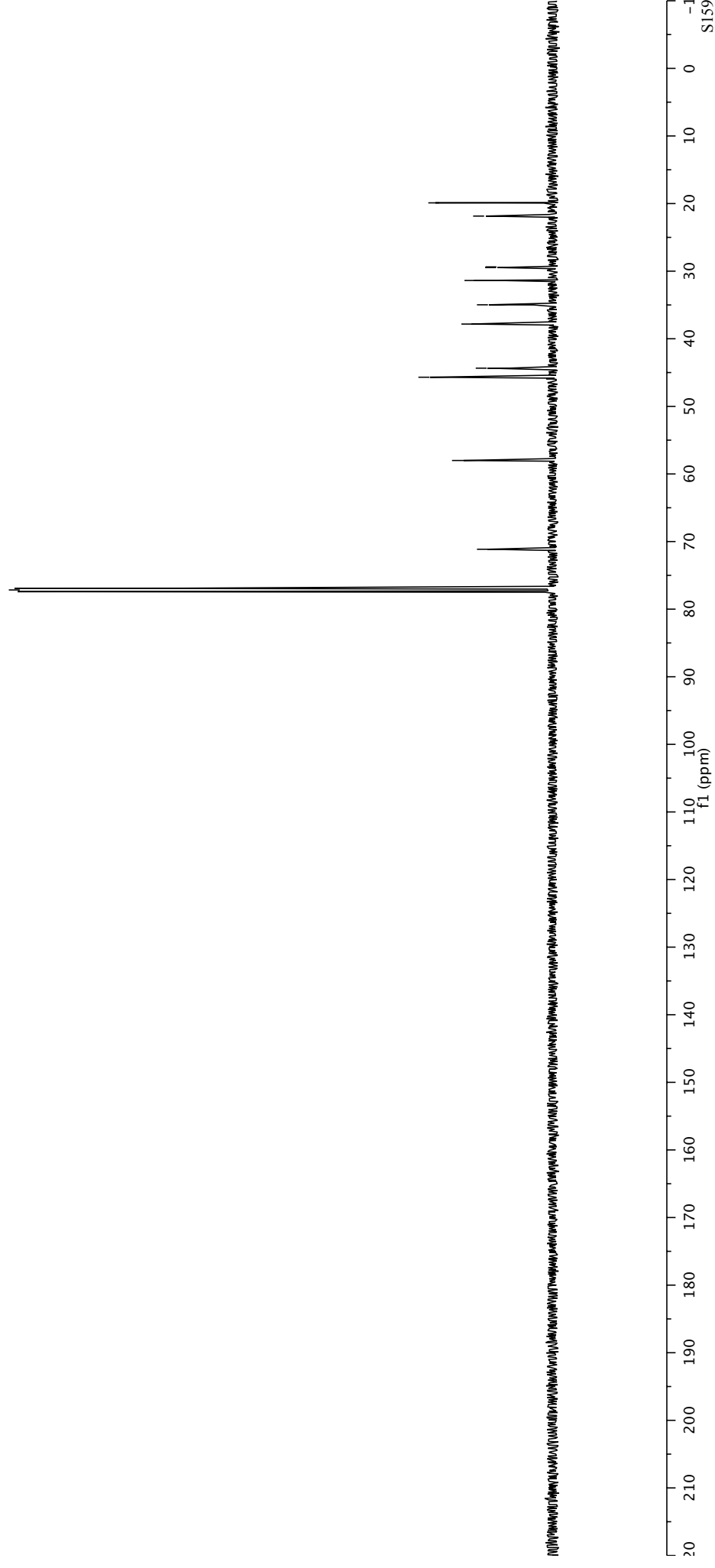
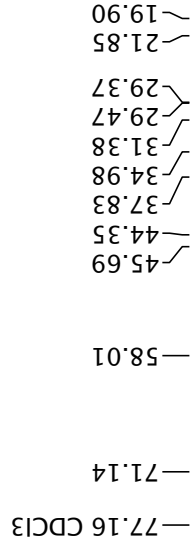
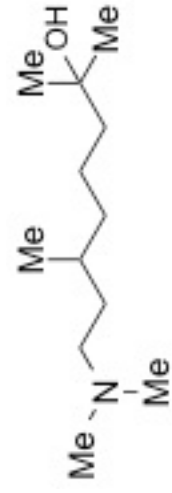
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	32
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1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





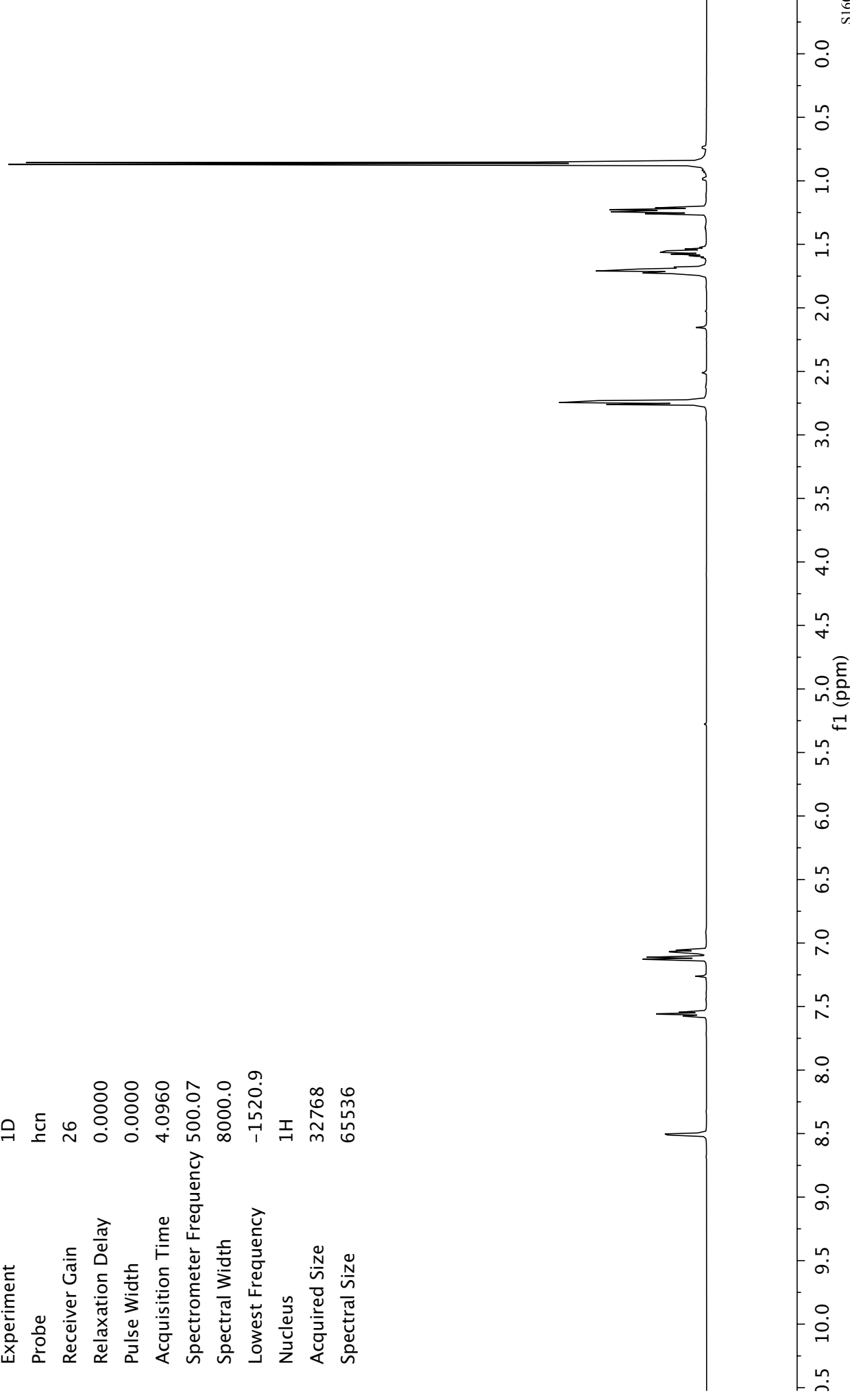
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Number of Scans	783
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2200.4
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

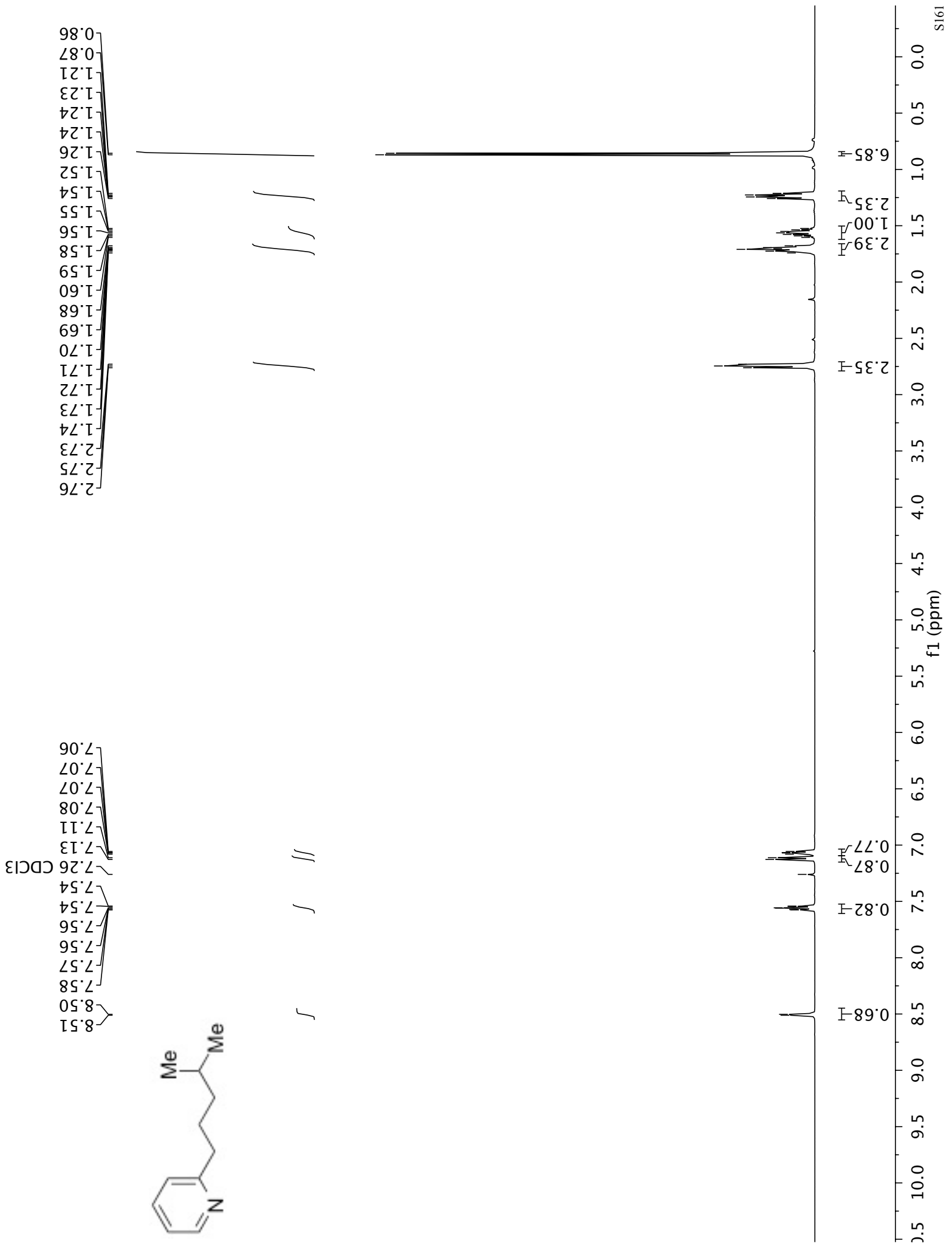






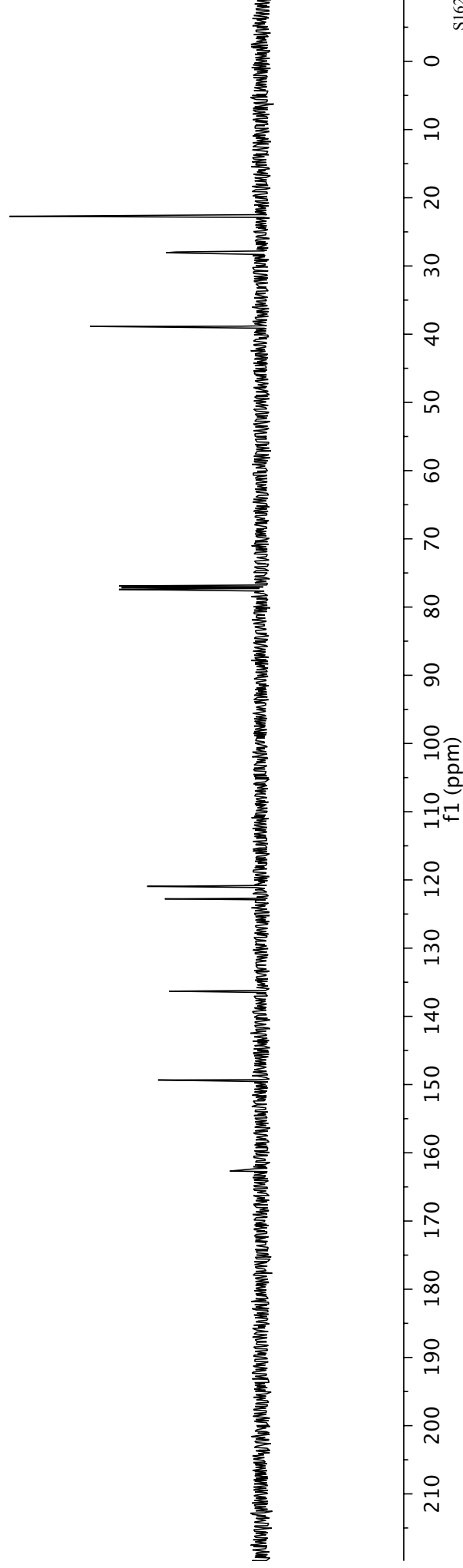
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	26
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1520.9
Nucleus	1H
Acquired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

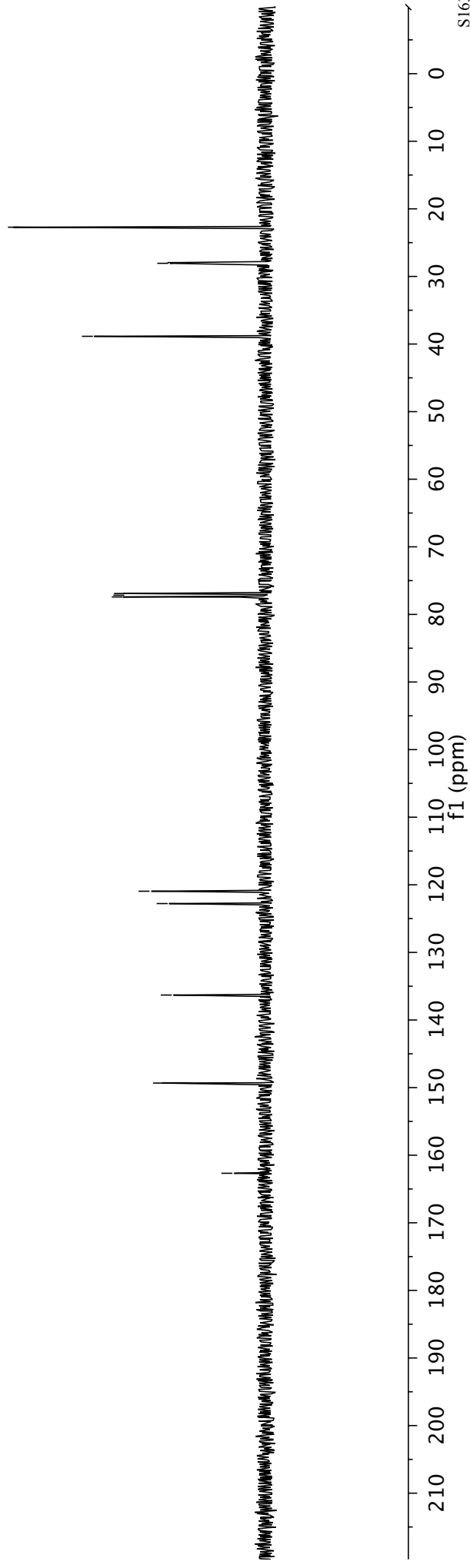






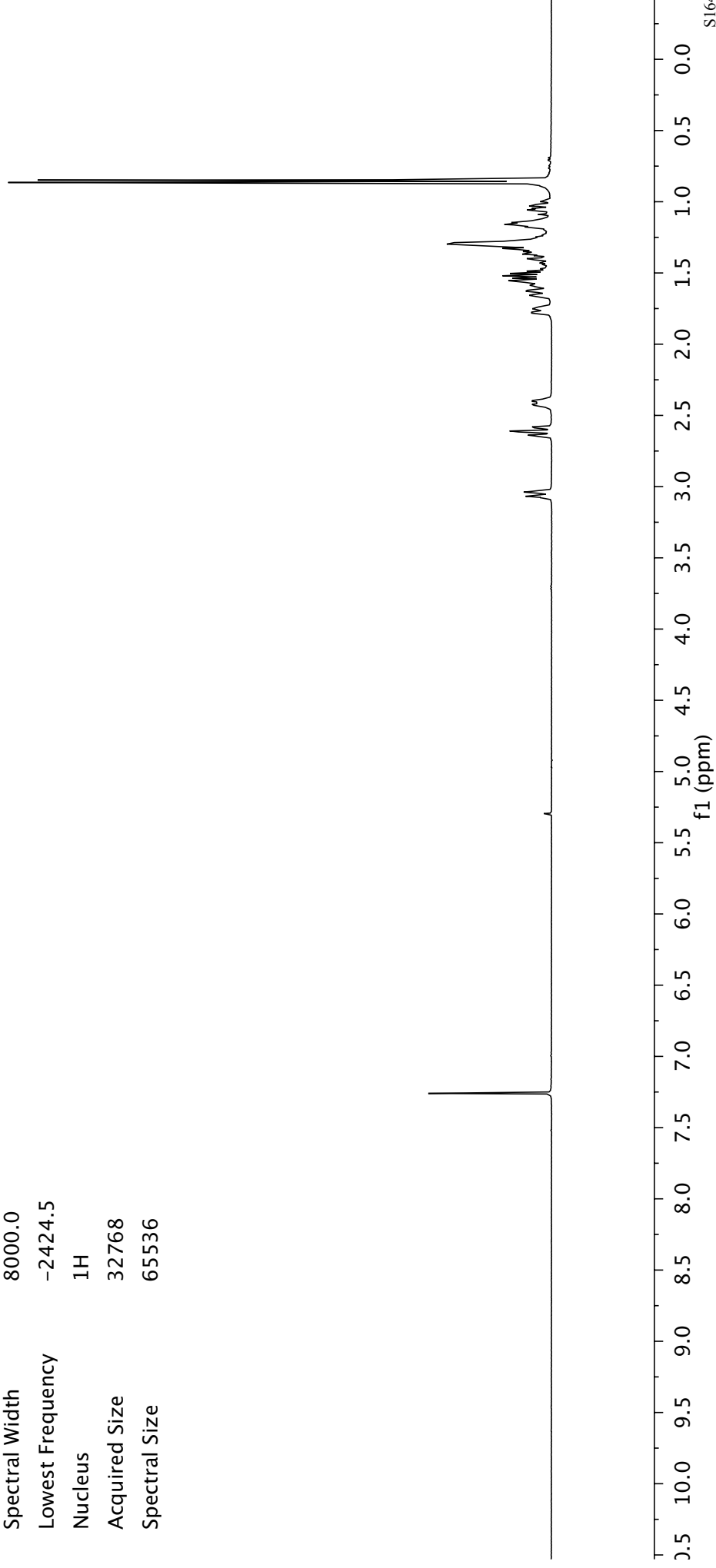
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2204.6
Nucleus	¹³ C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



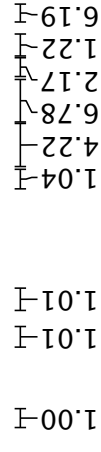
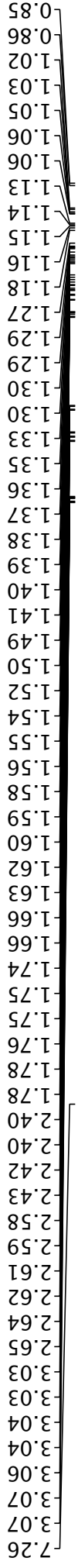
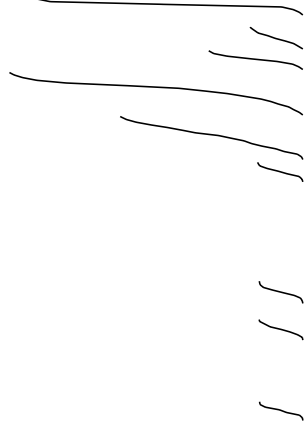




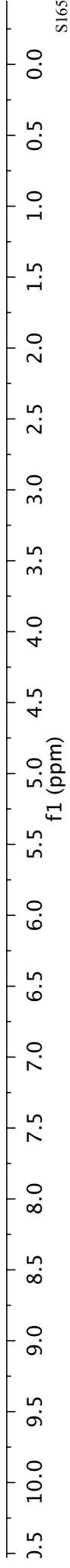
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	54
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	399.95
Spectral Width	8000.0
Lowest Frequency	-2424.5
Nucleus	1H
Acquired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

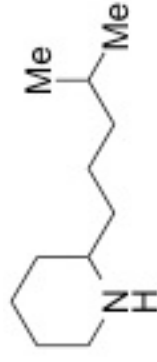


7.26 CDCl₃

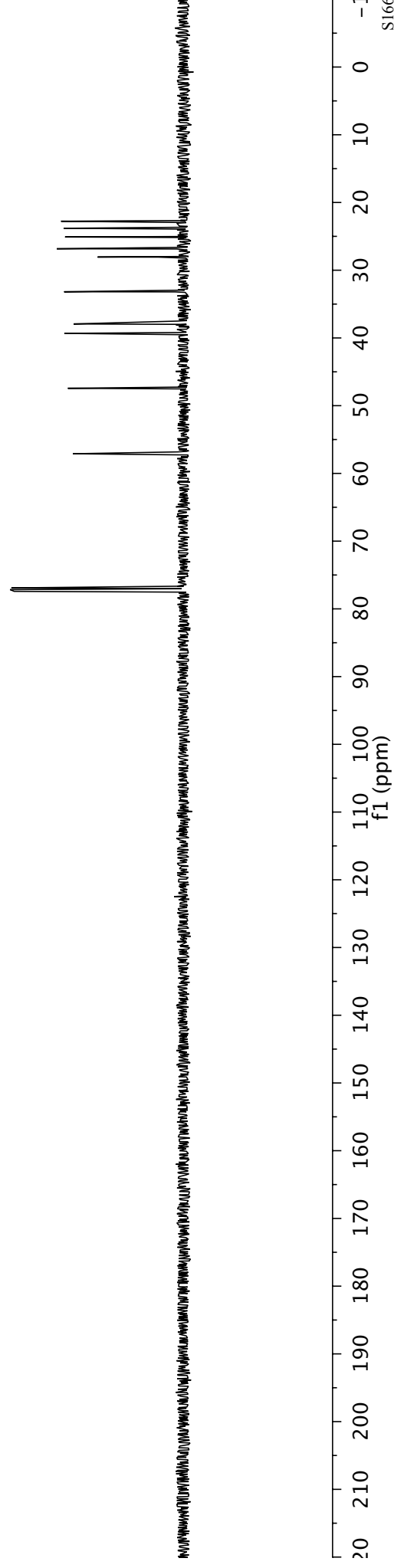


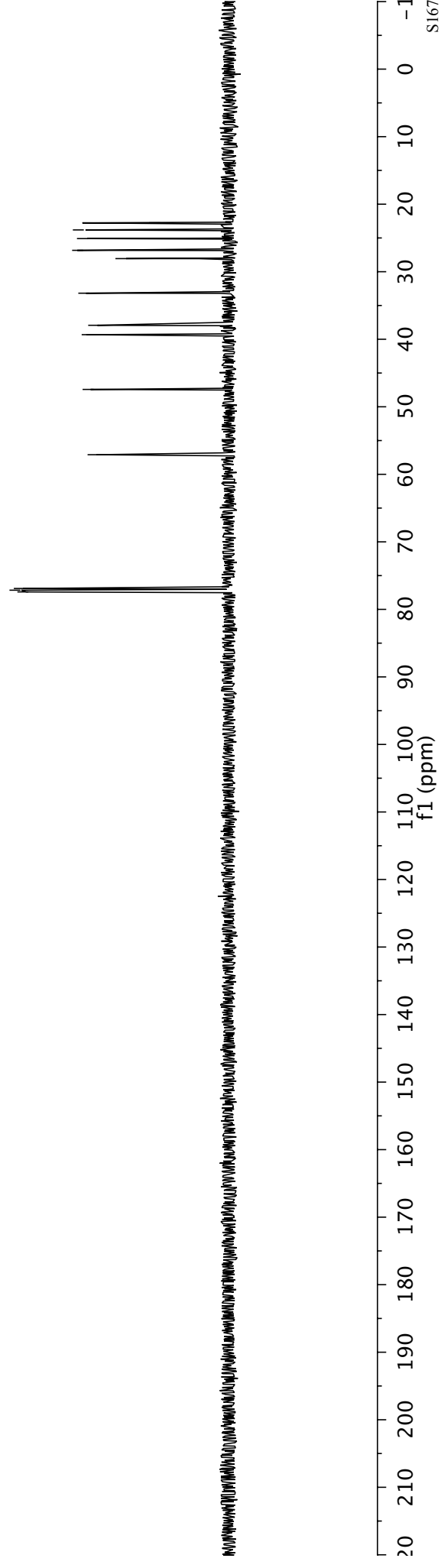
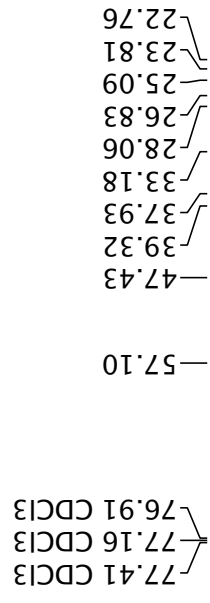
f1 (ppm)

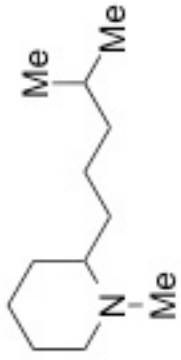




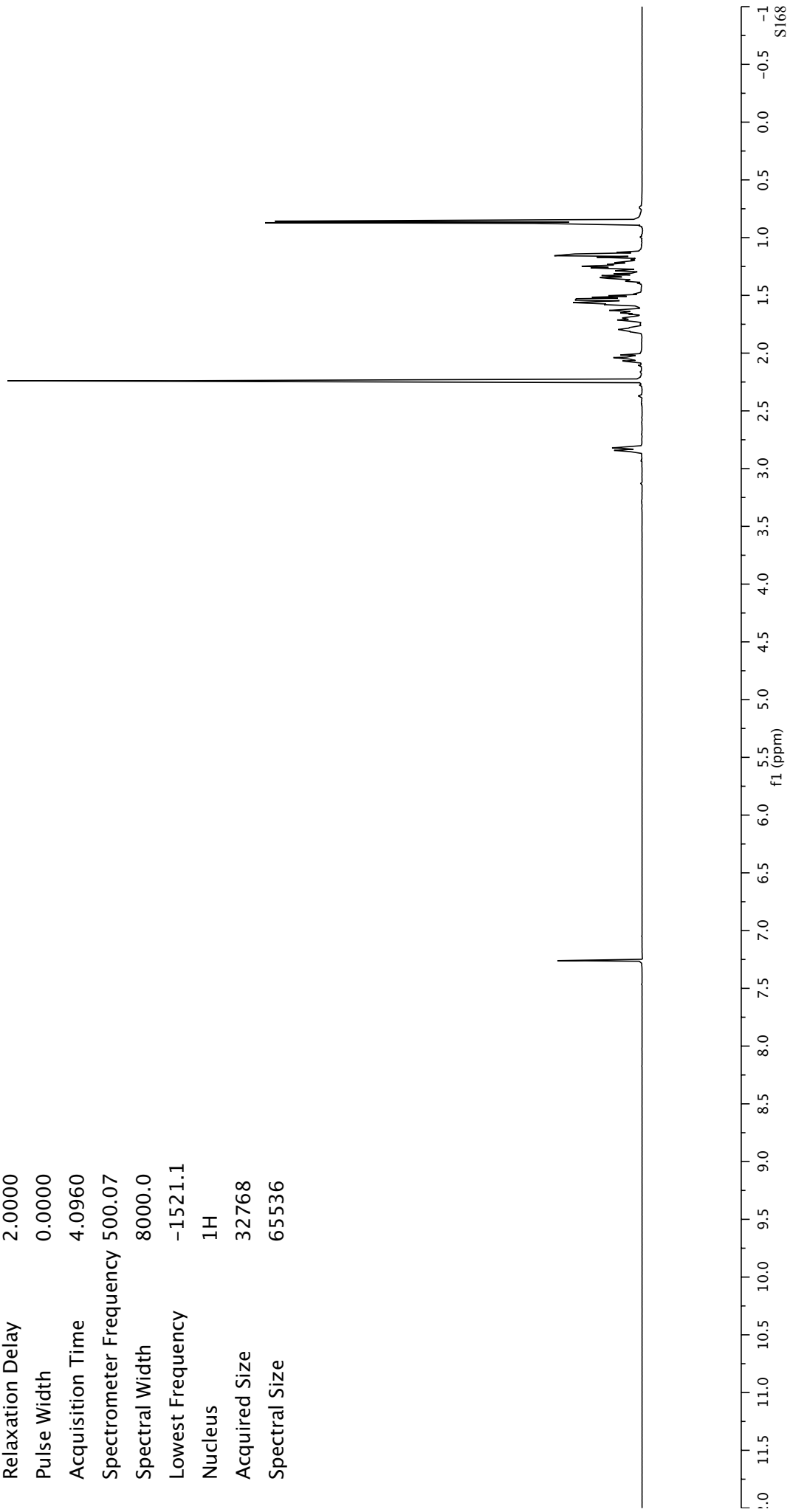
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1272.5
Nucleus	¹³ C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

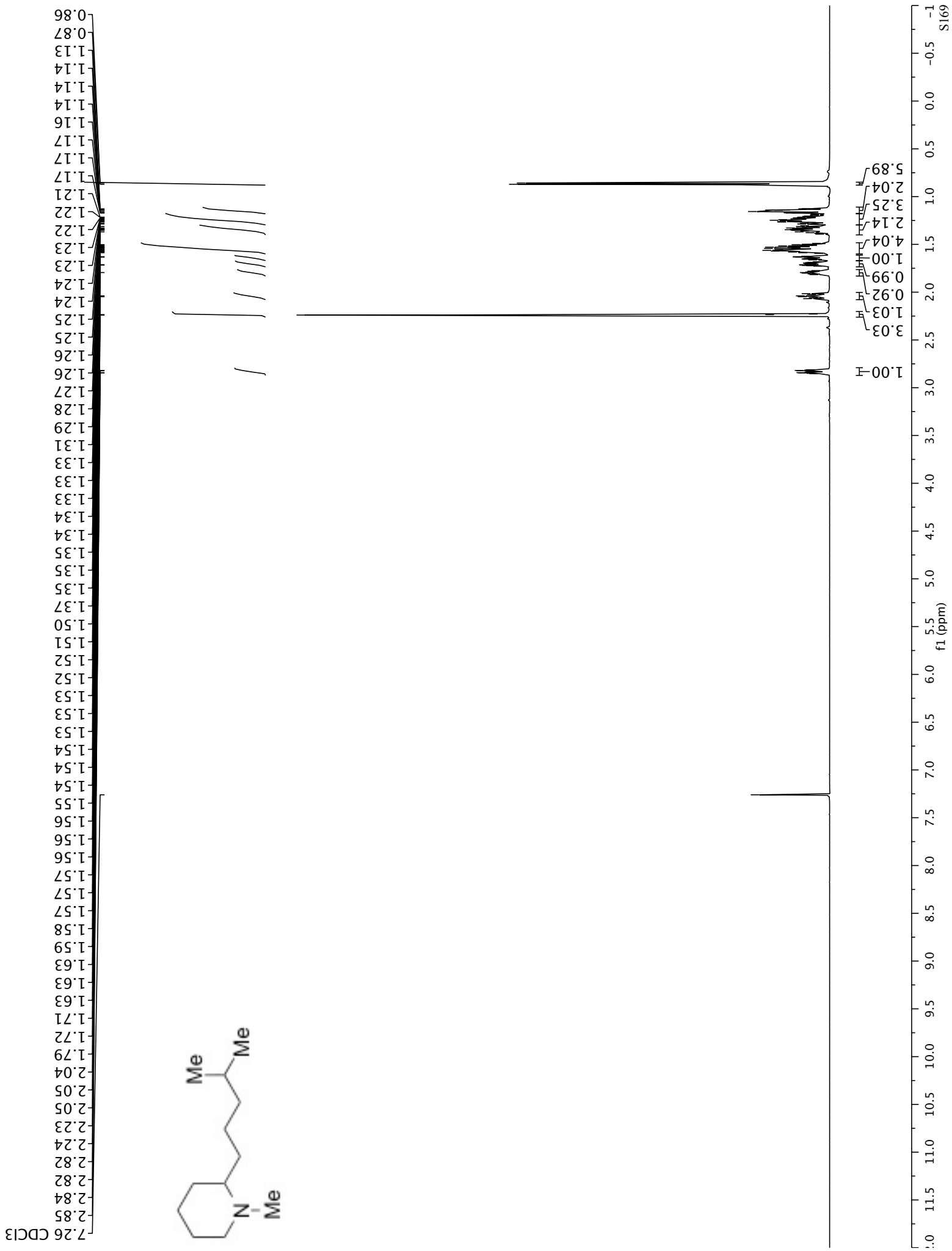
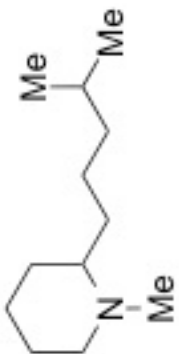


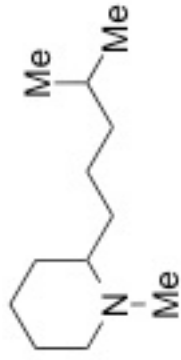




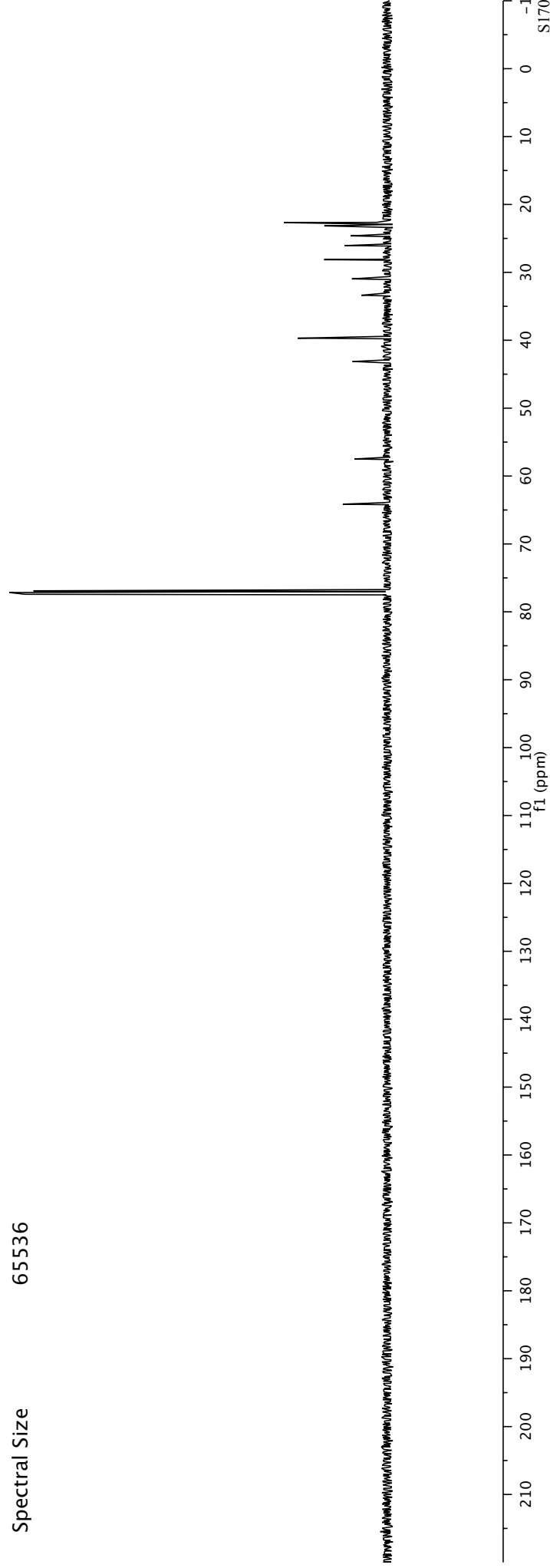
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	32
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1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

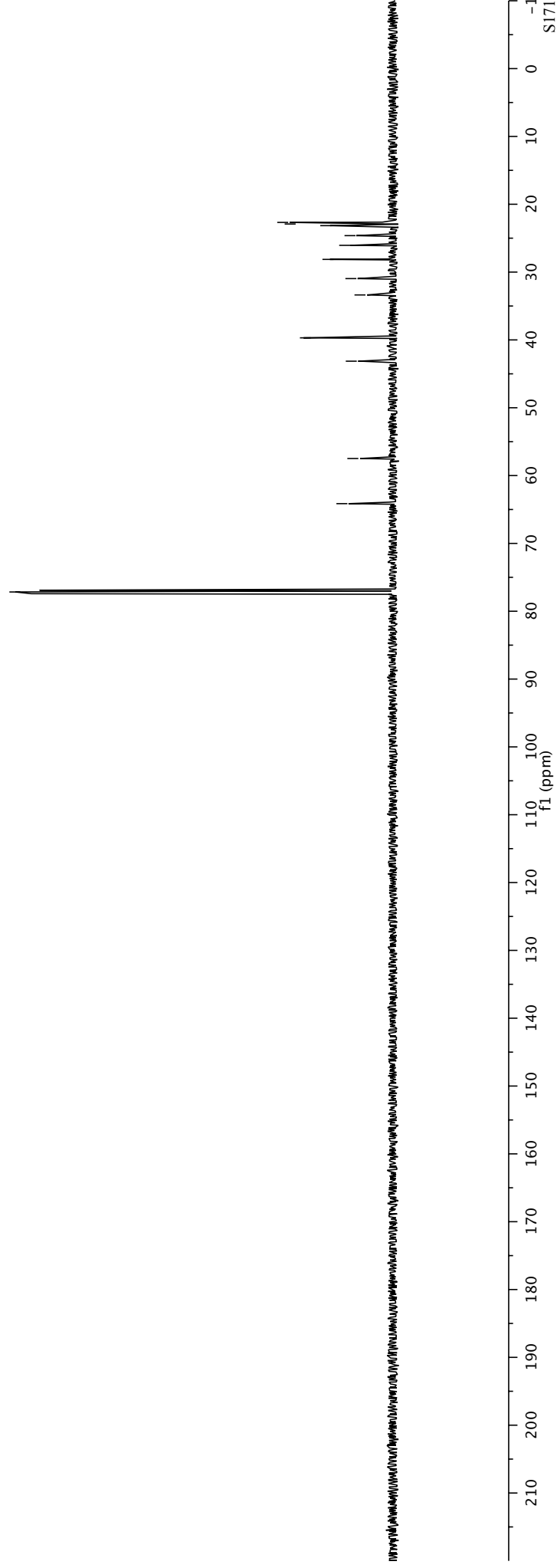
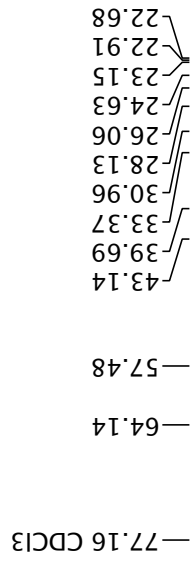
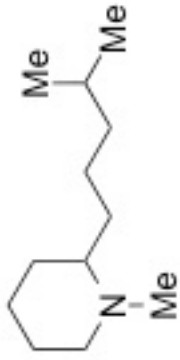




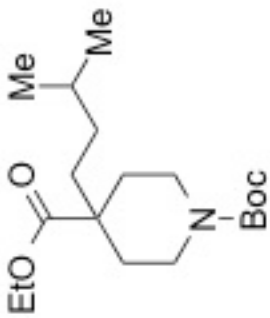


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Number of Scans	704
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency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

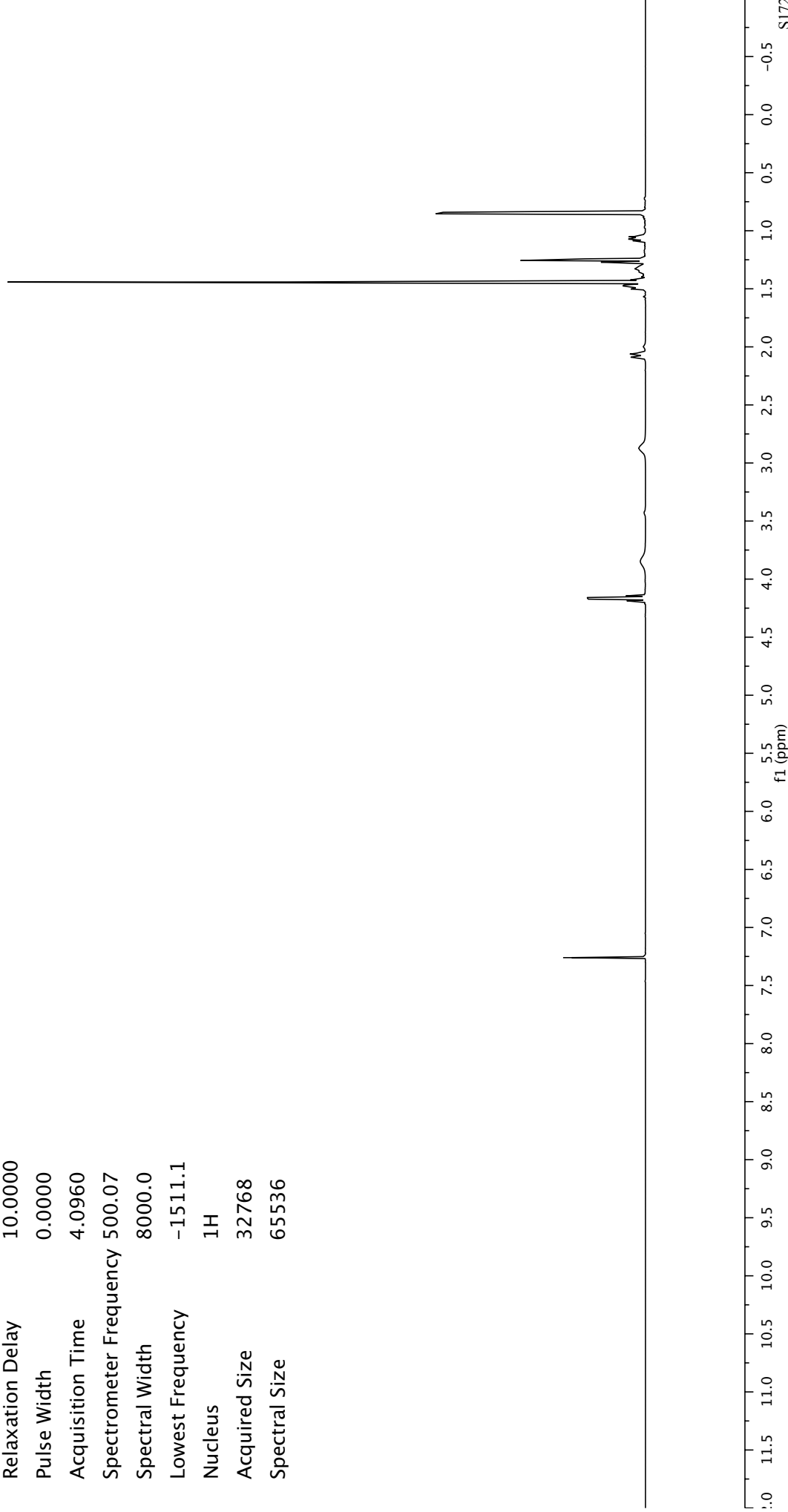


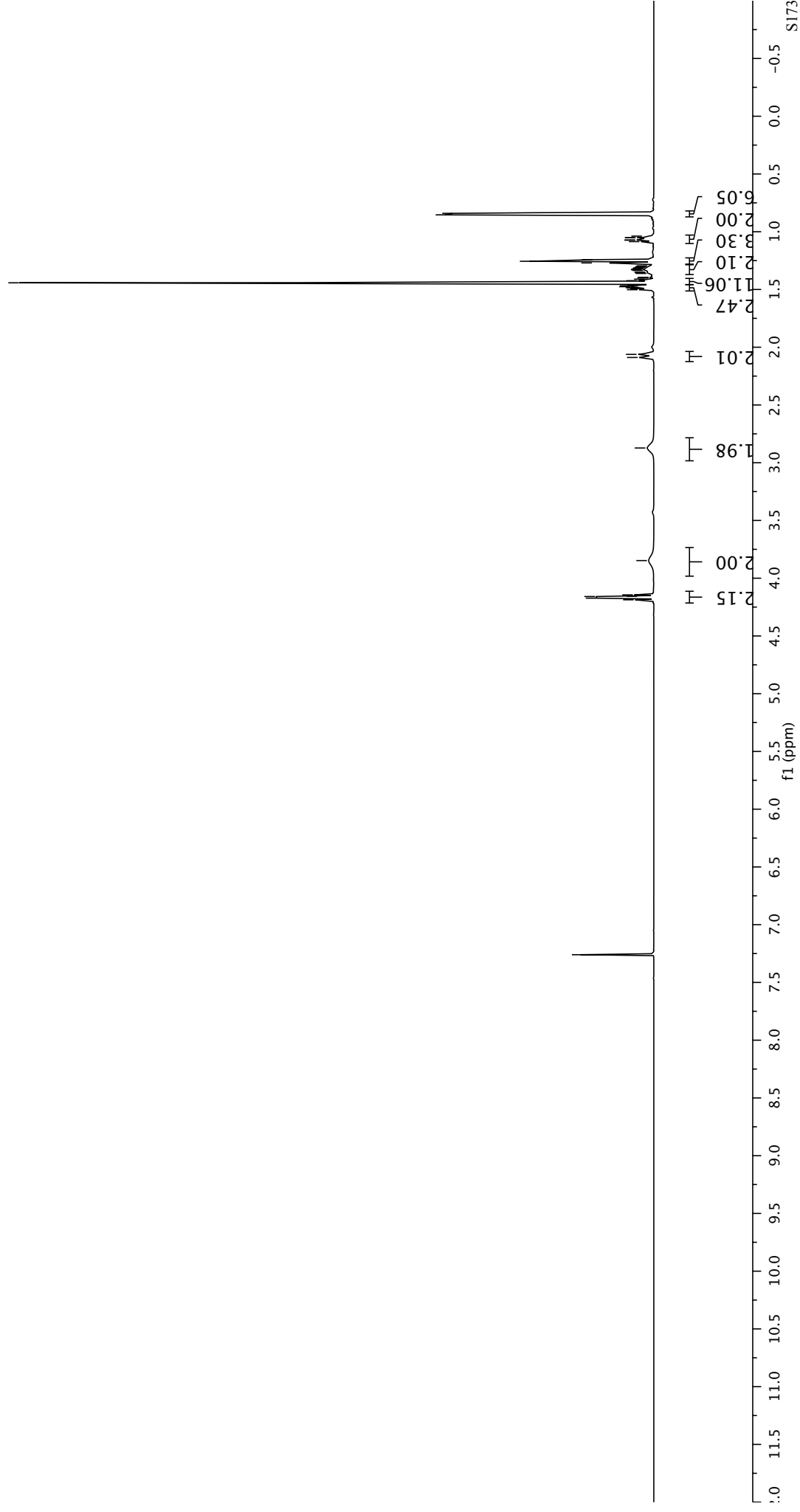
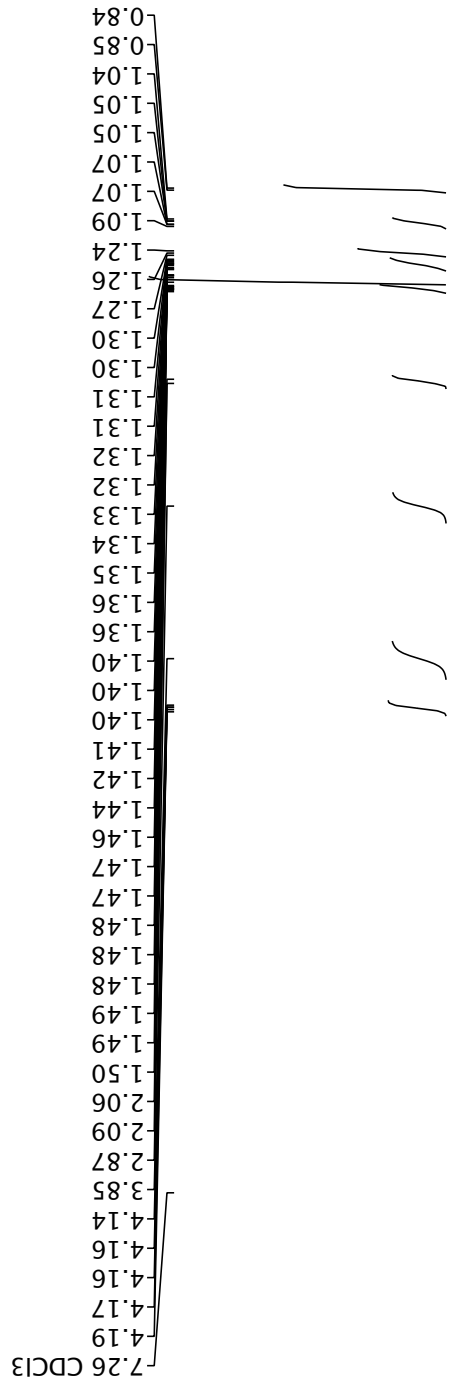
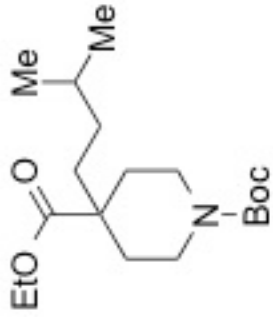


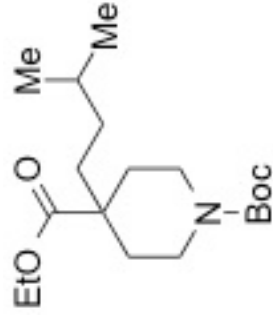
—7.26 CDCl₃



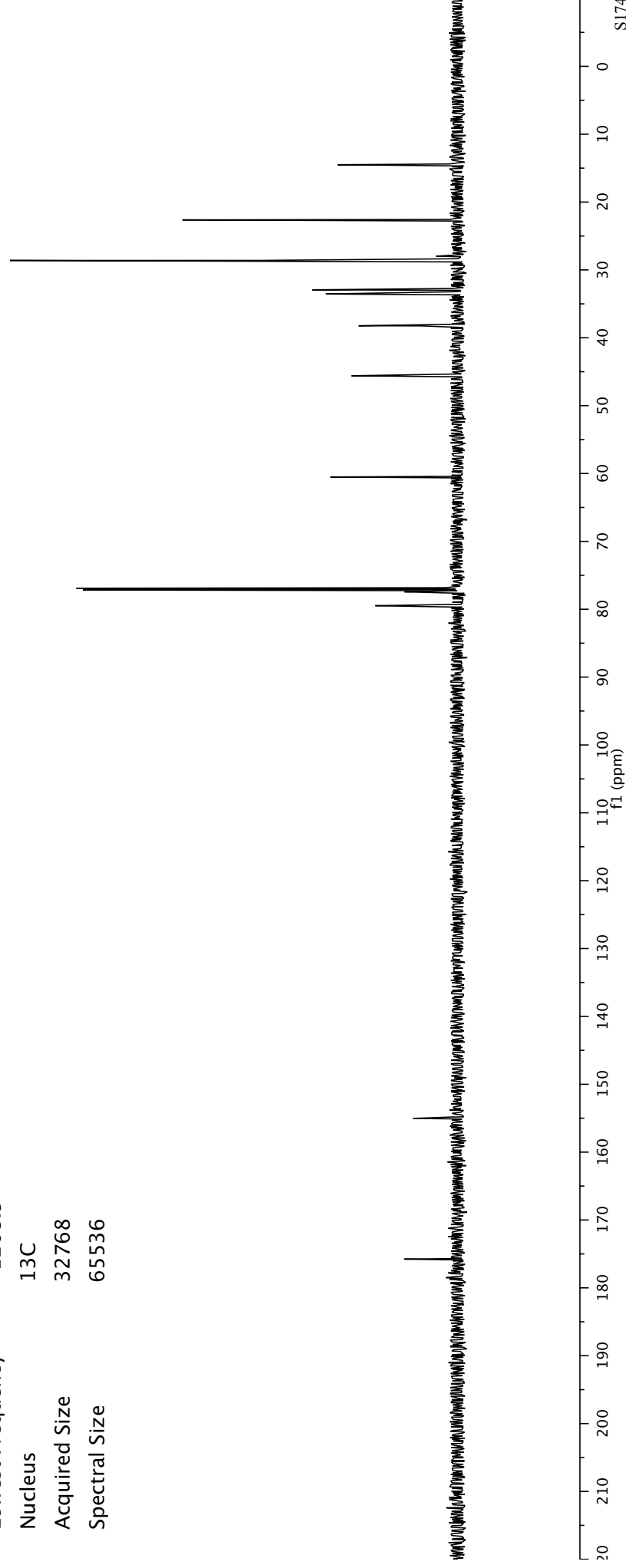
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	32
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1511.1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

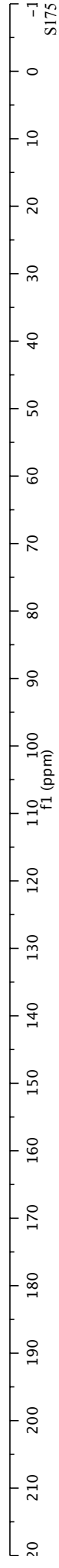
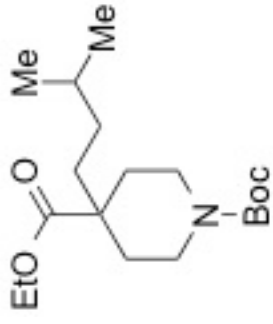


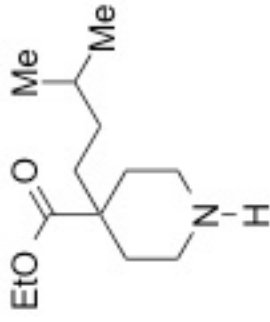




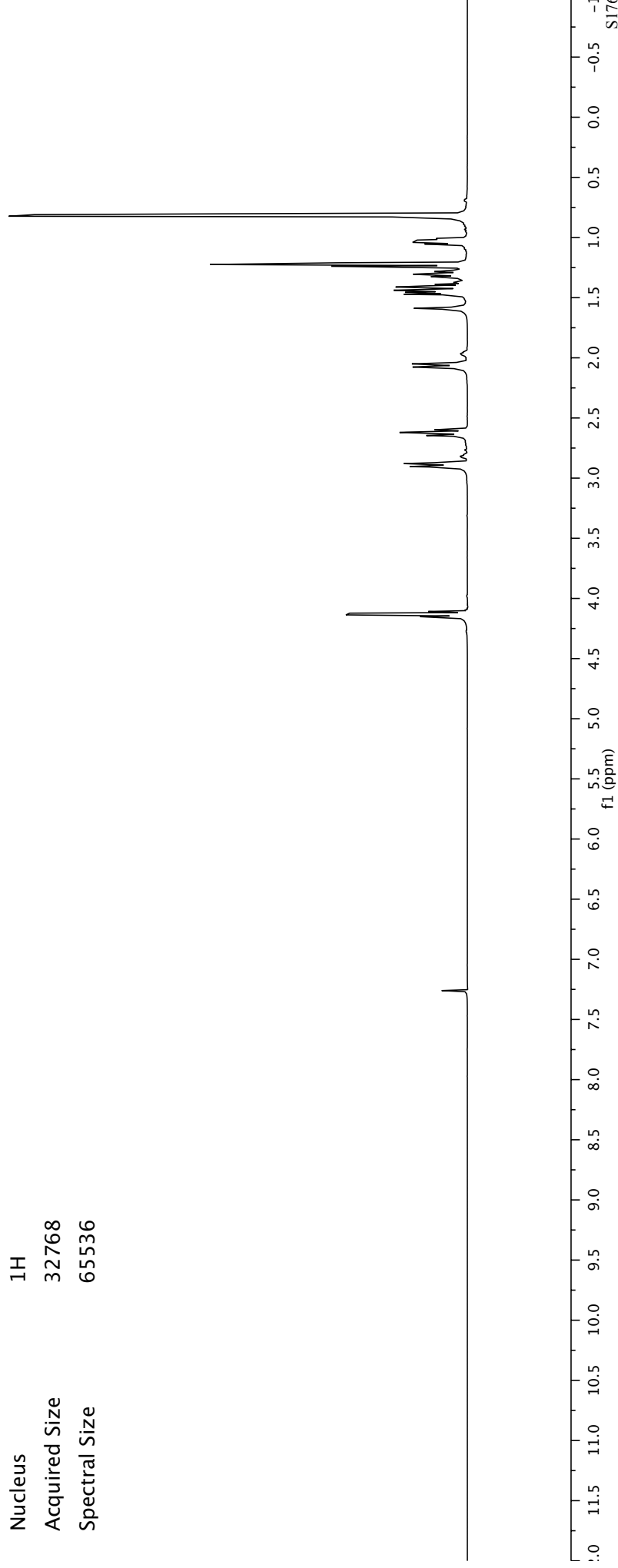
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	35.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	296
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1268.5
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

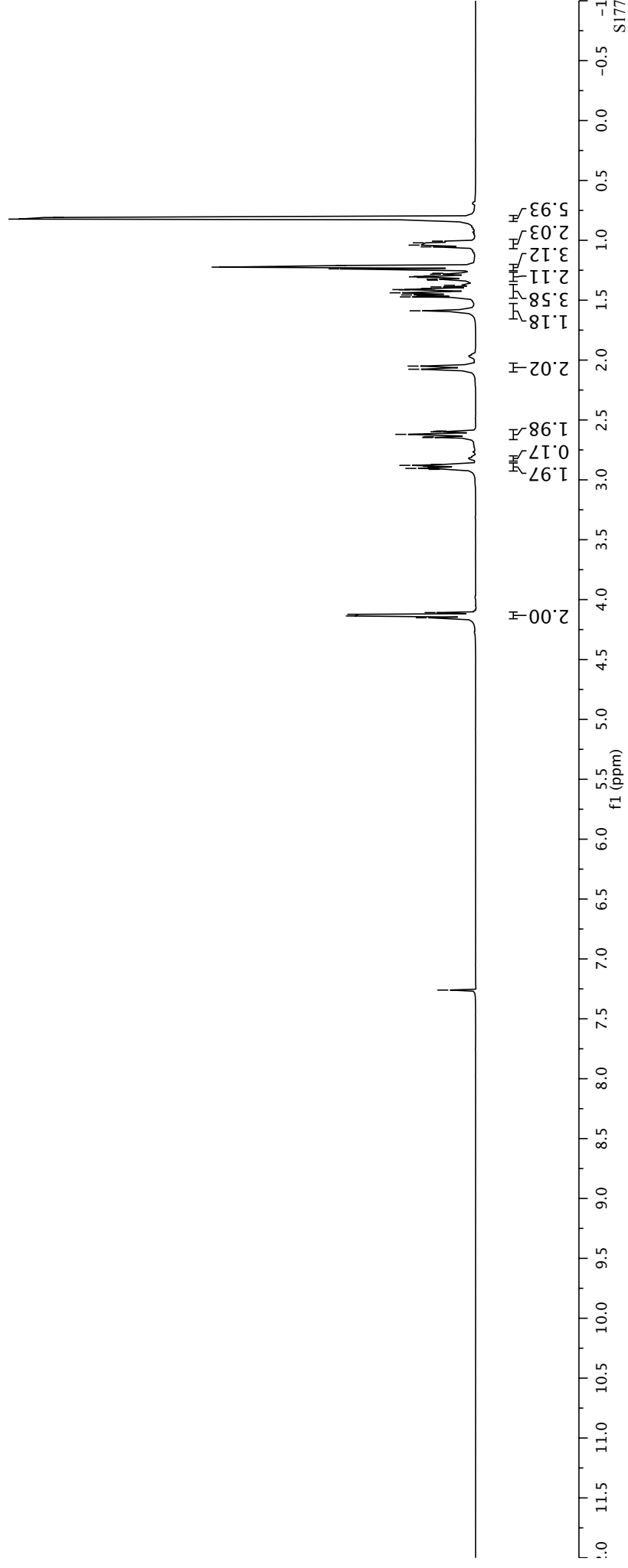
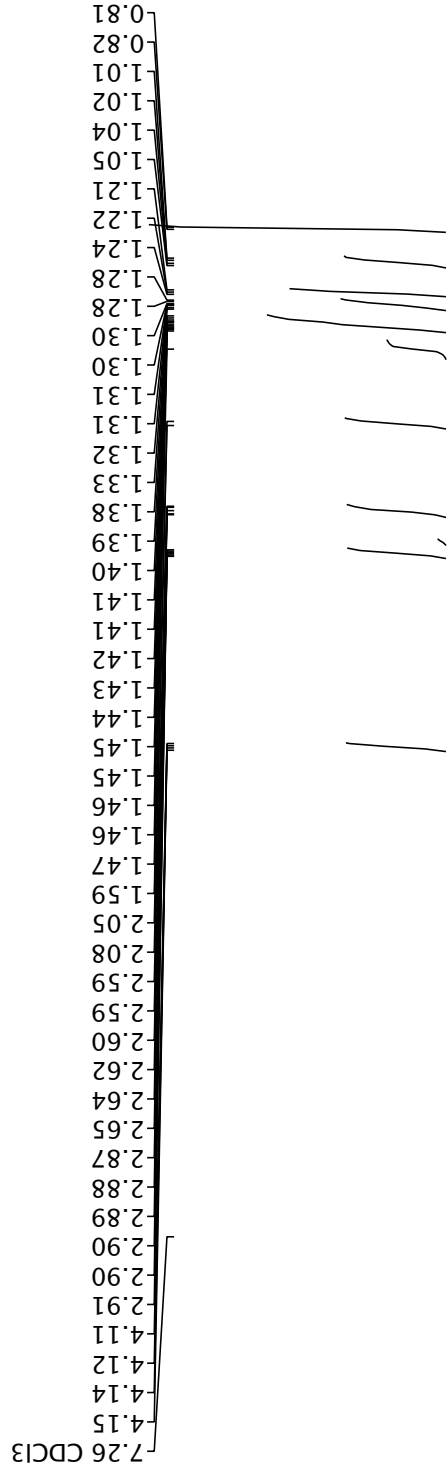
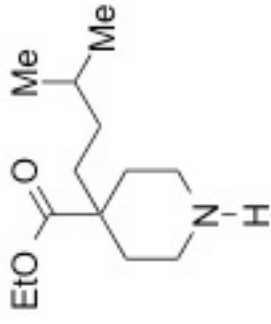


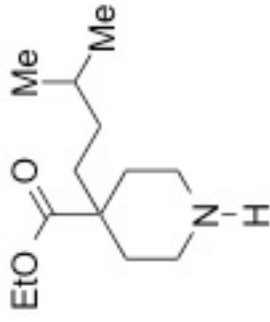




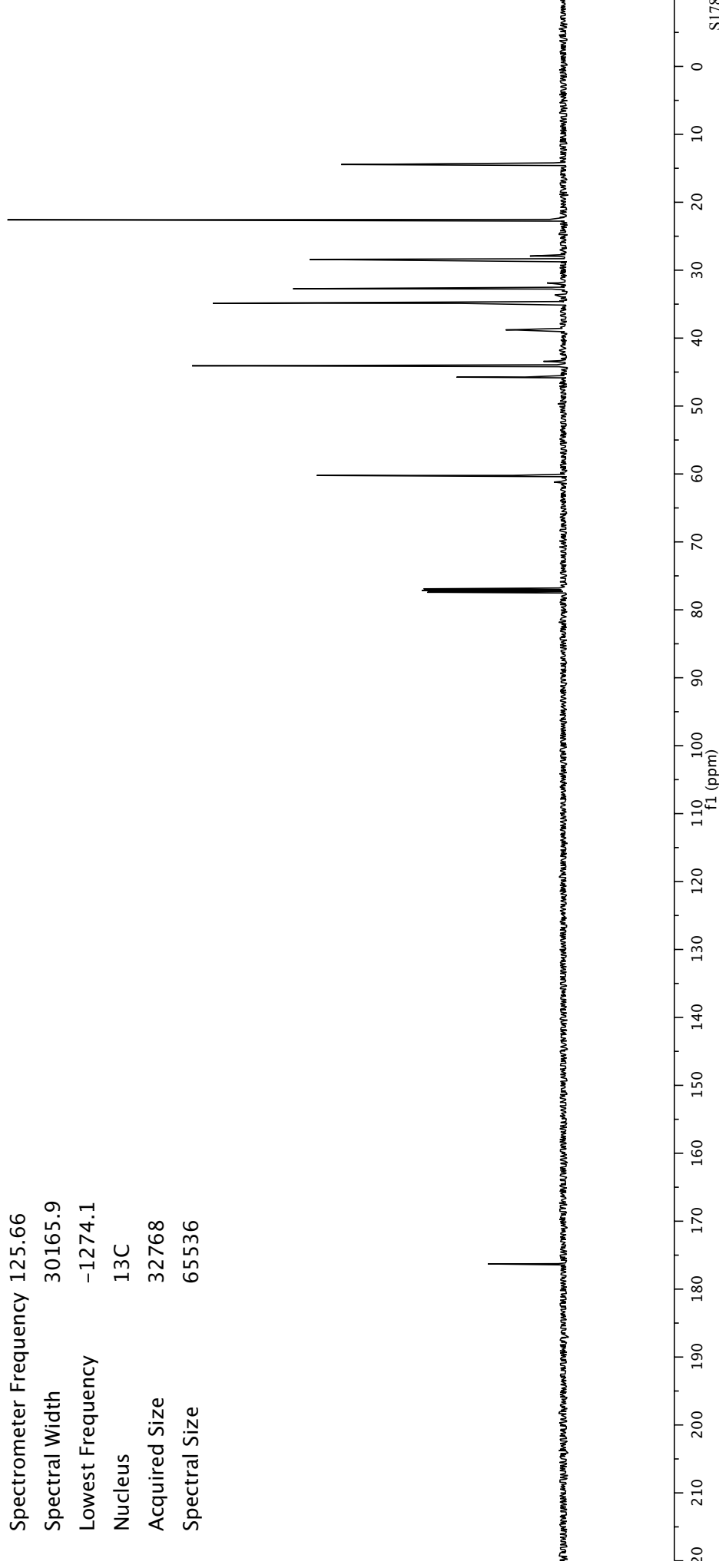
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	21.1
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	20
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1510.6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

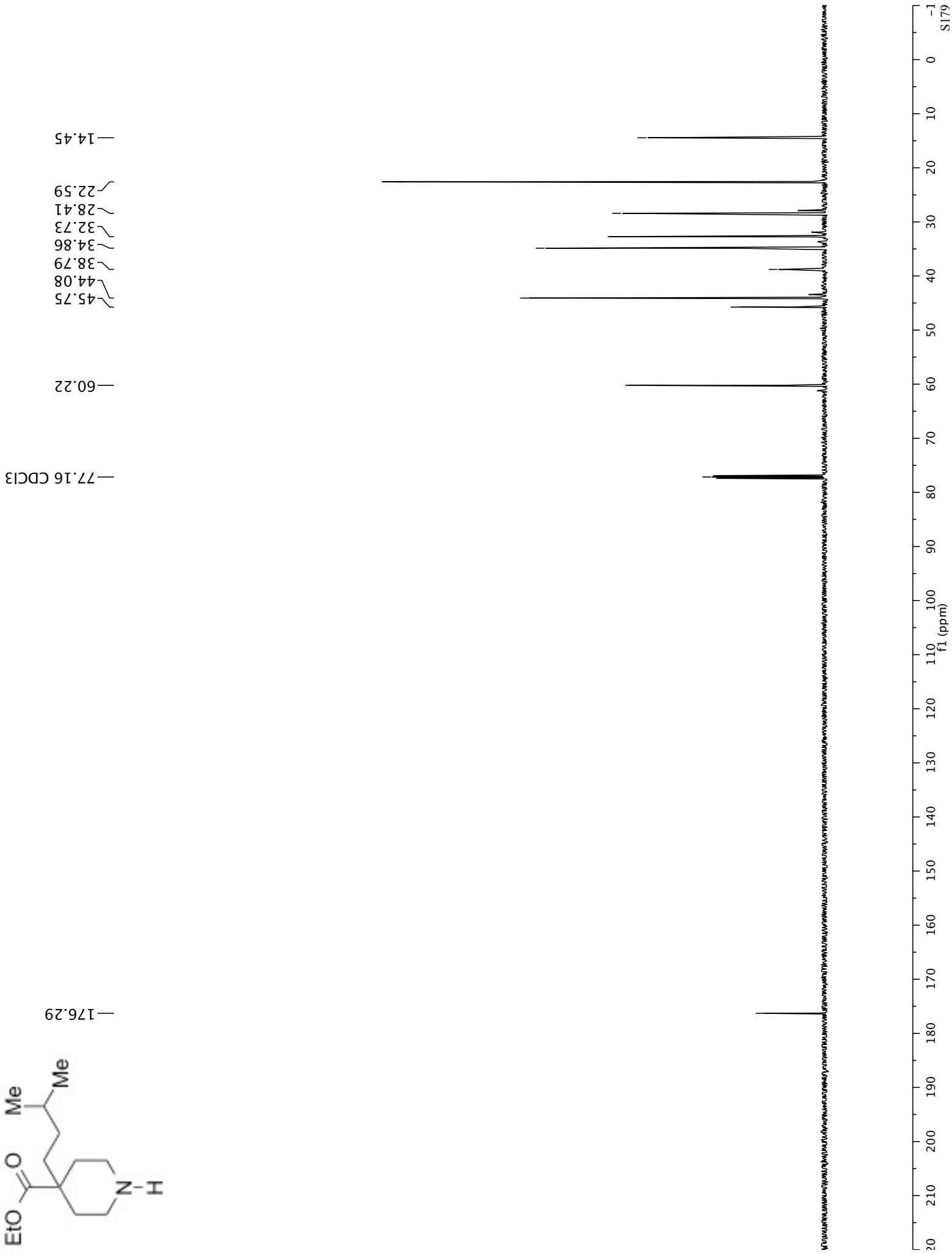
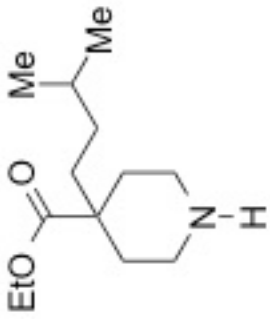


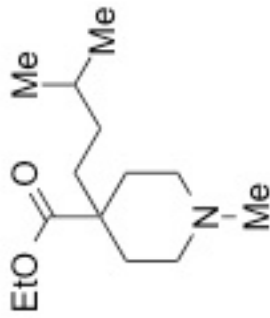




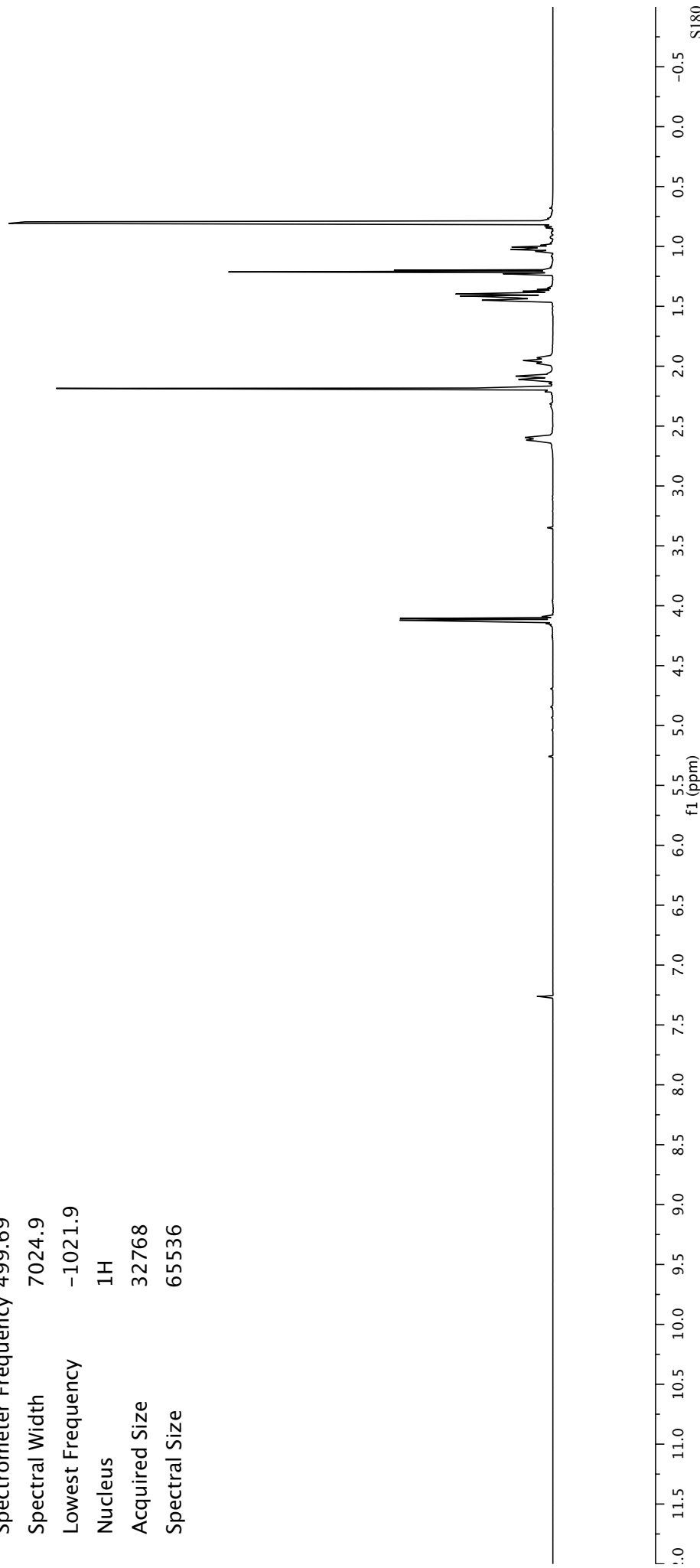
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	241
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1274.1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

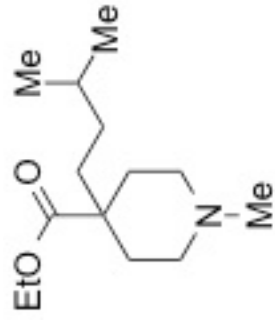




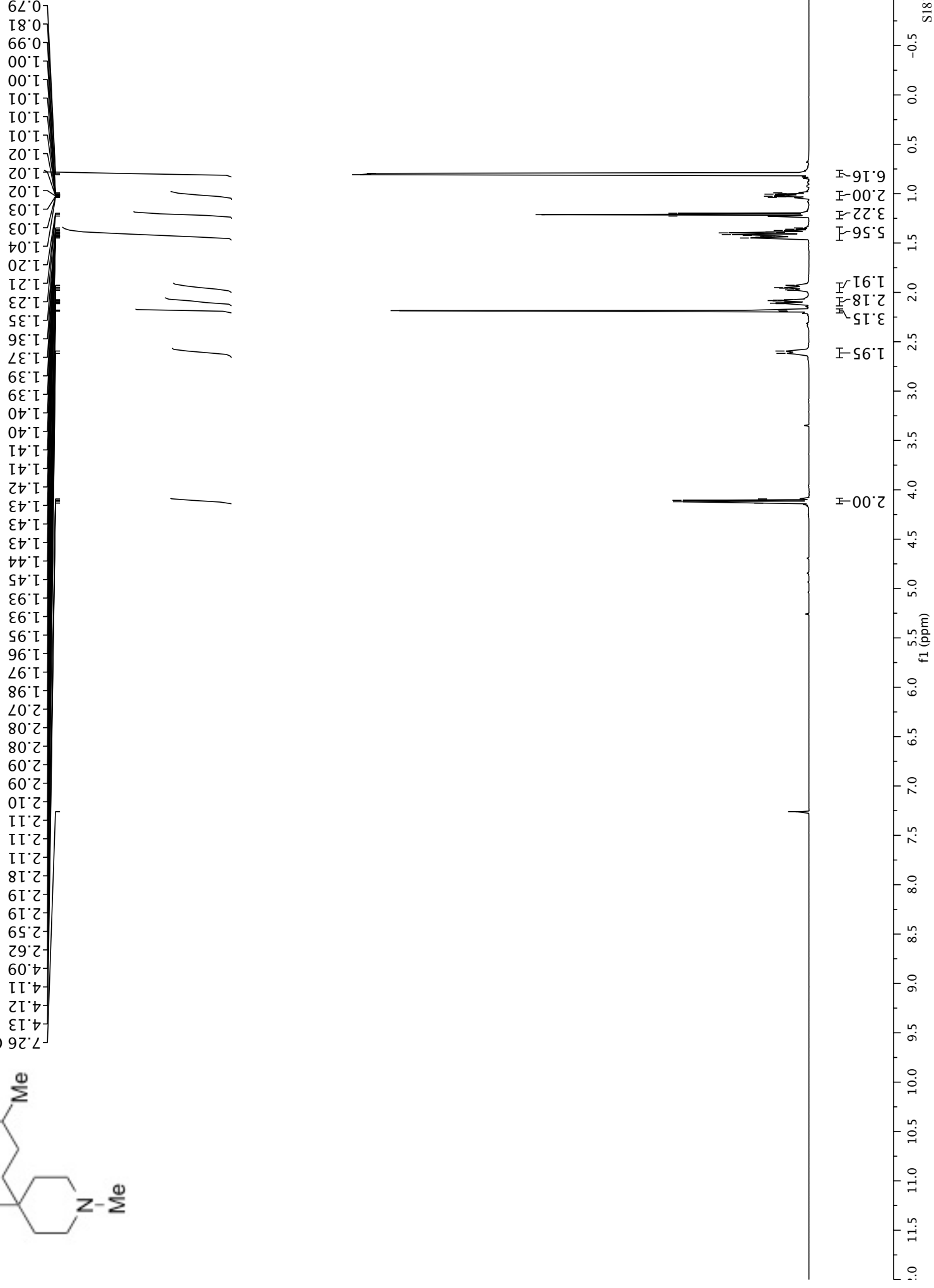


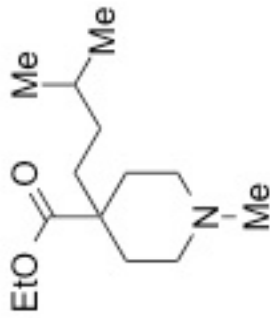
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	8
Receiver Gain	30
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.69
Spectral Width	7024.9
Lowest Frequency	-1021.9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



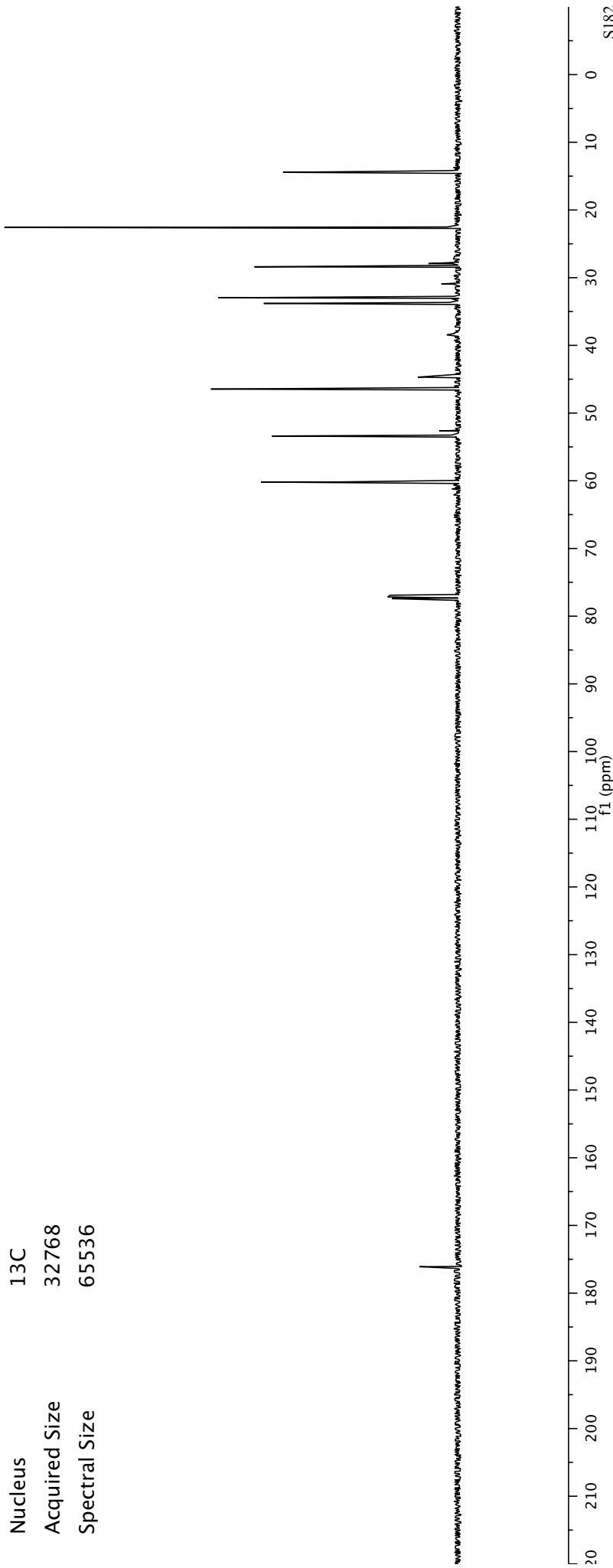


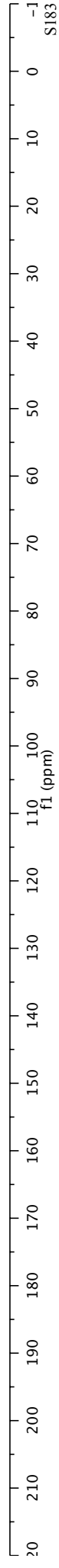
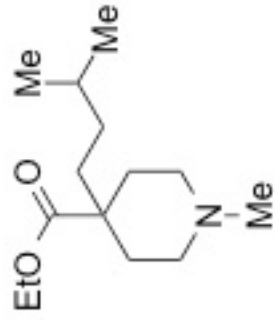
7.26 CDCl₃

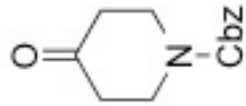




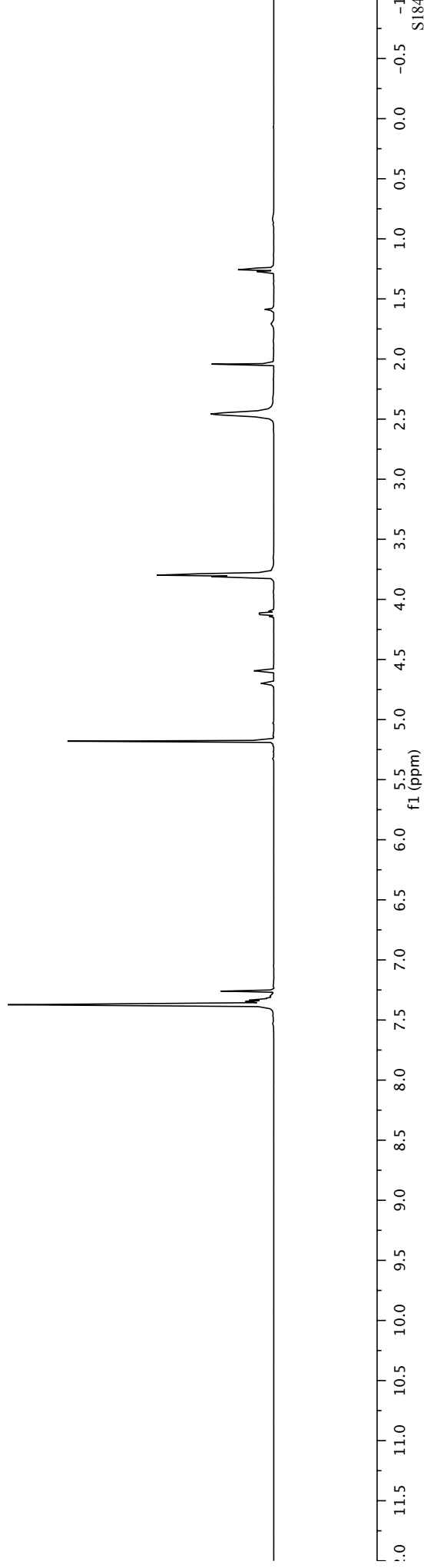
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	80
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1276.3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

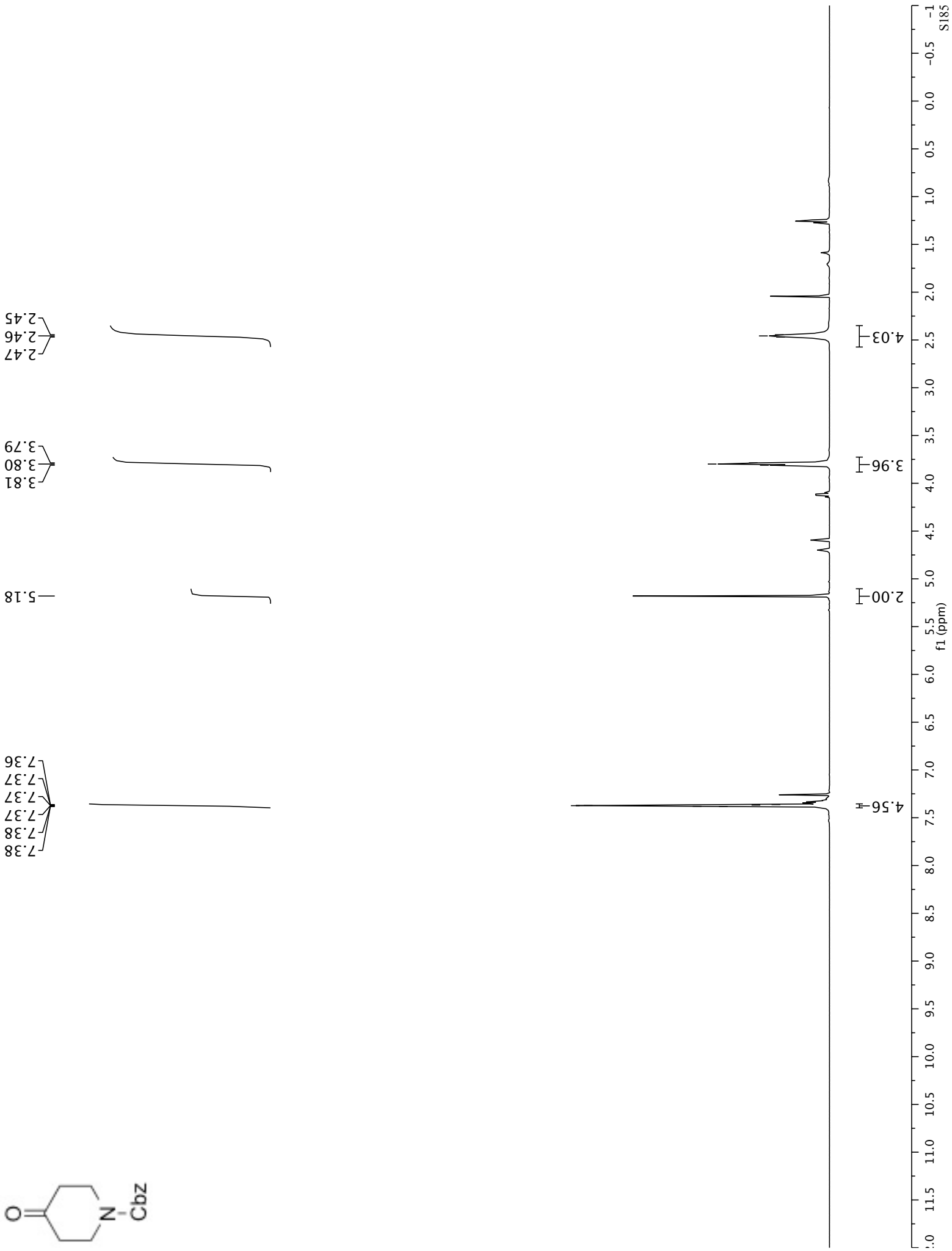
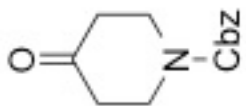


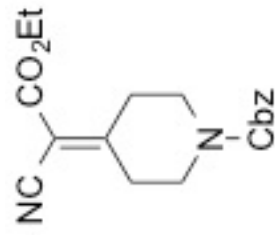




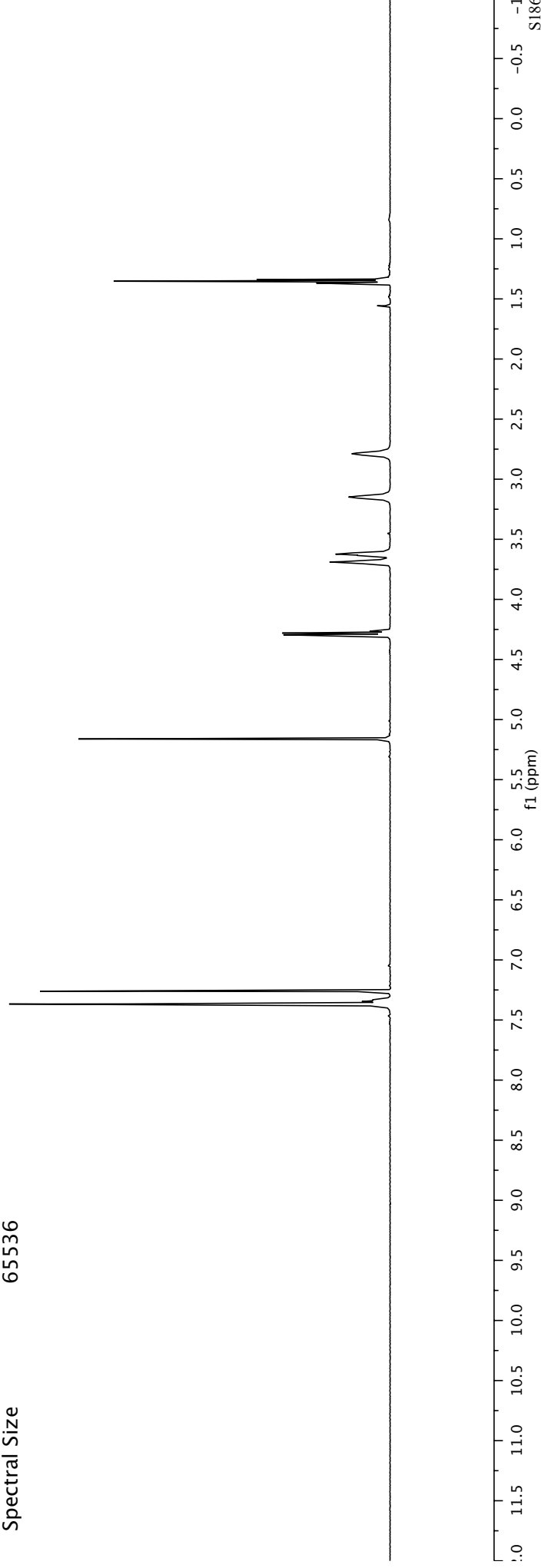
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	8
Receiver Gain	36
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1510.6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

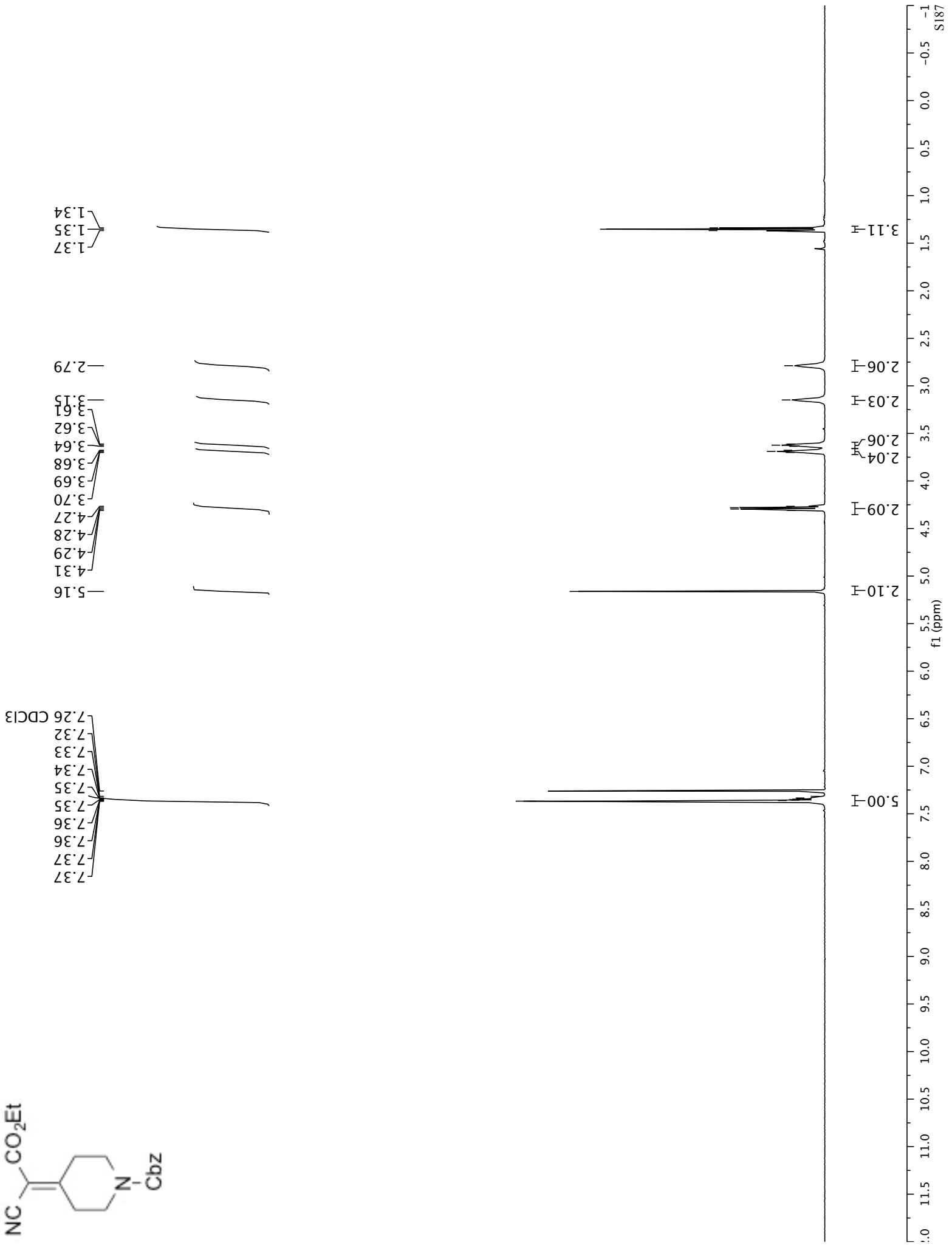
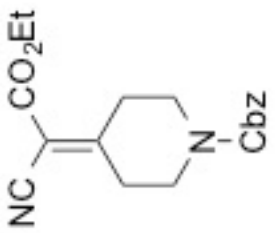


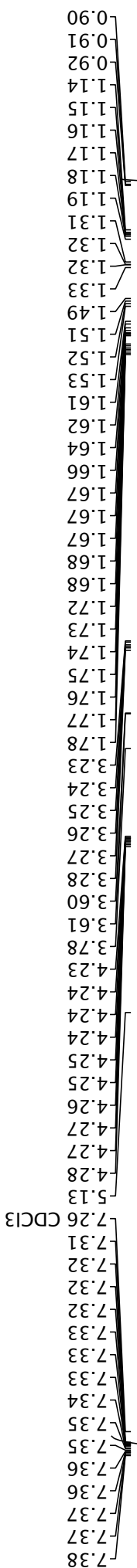
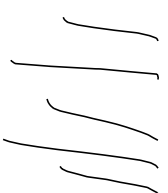
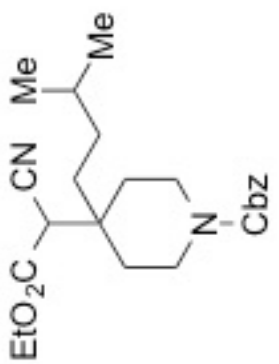
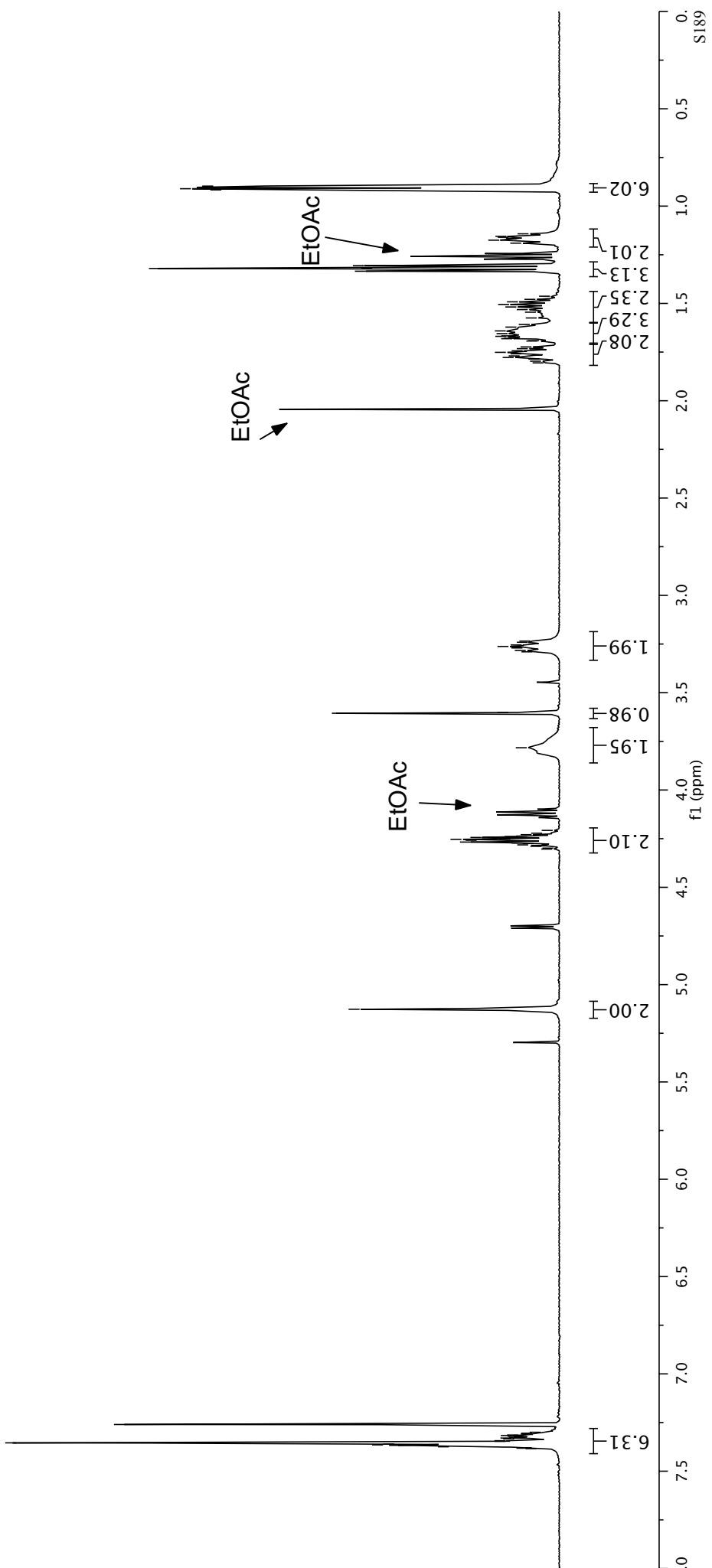


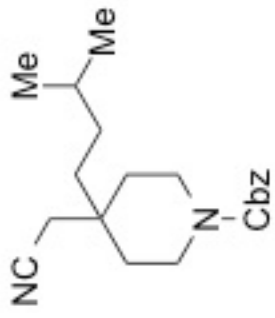


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	16
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.69
Spectral Width	7024.9
Lowest Frequency	-1011.4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

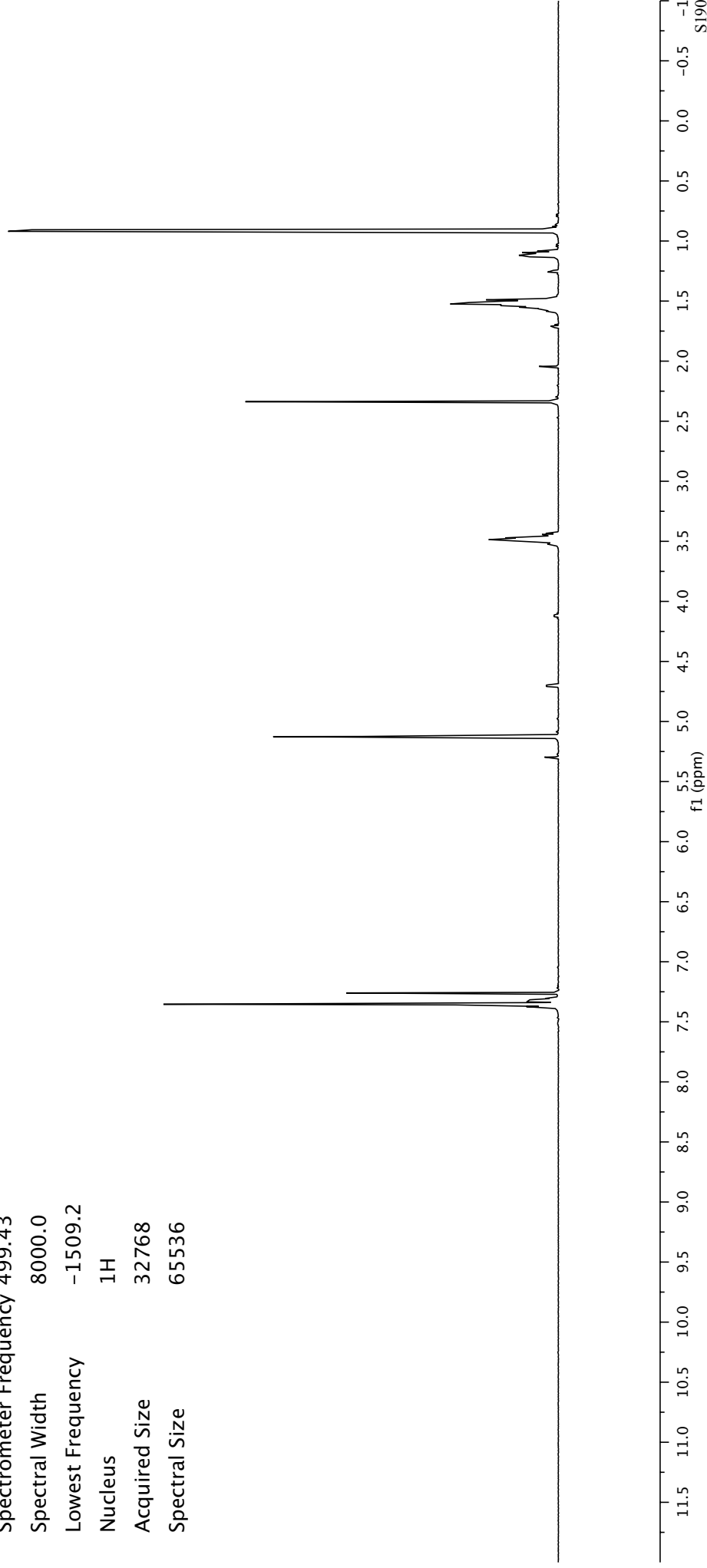


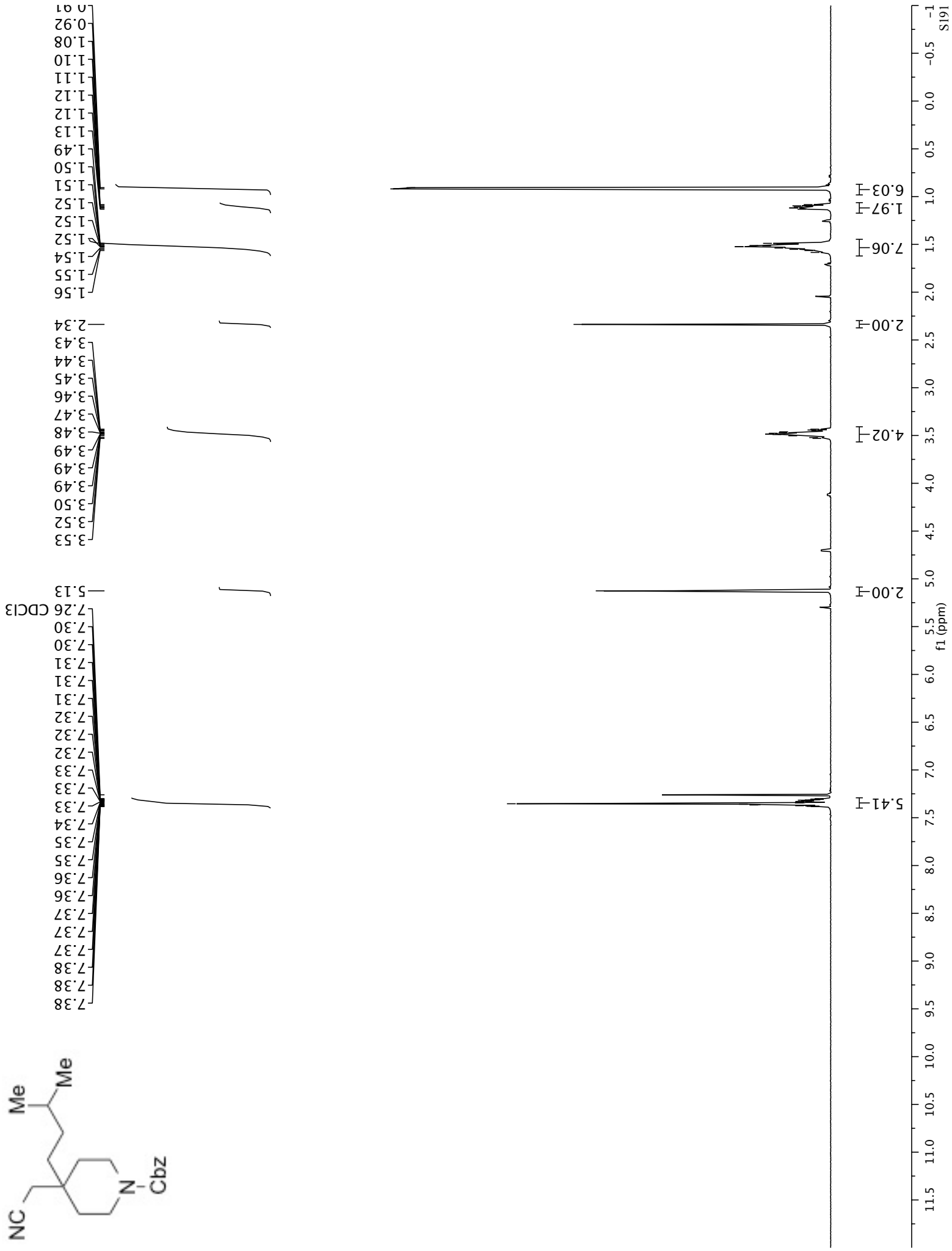
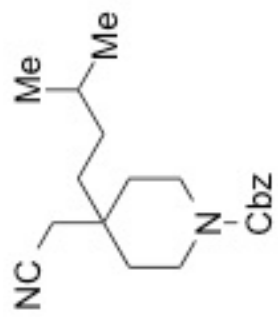


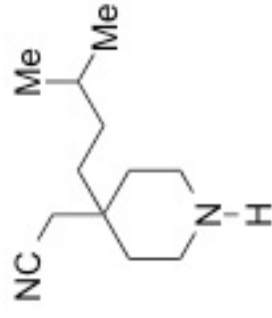




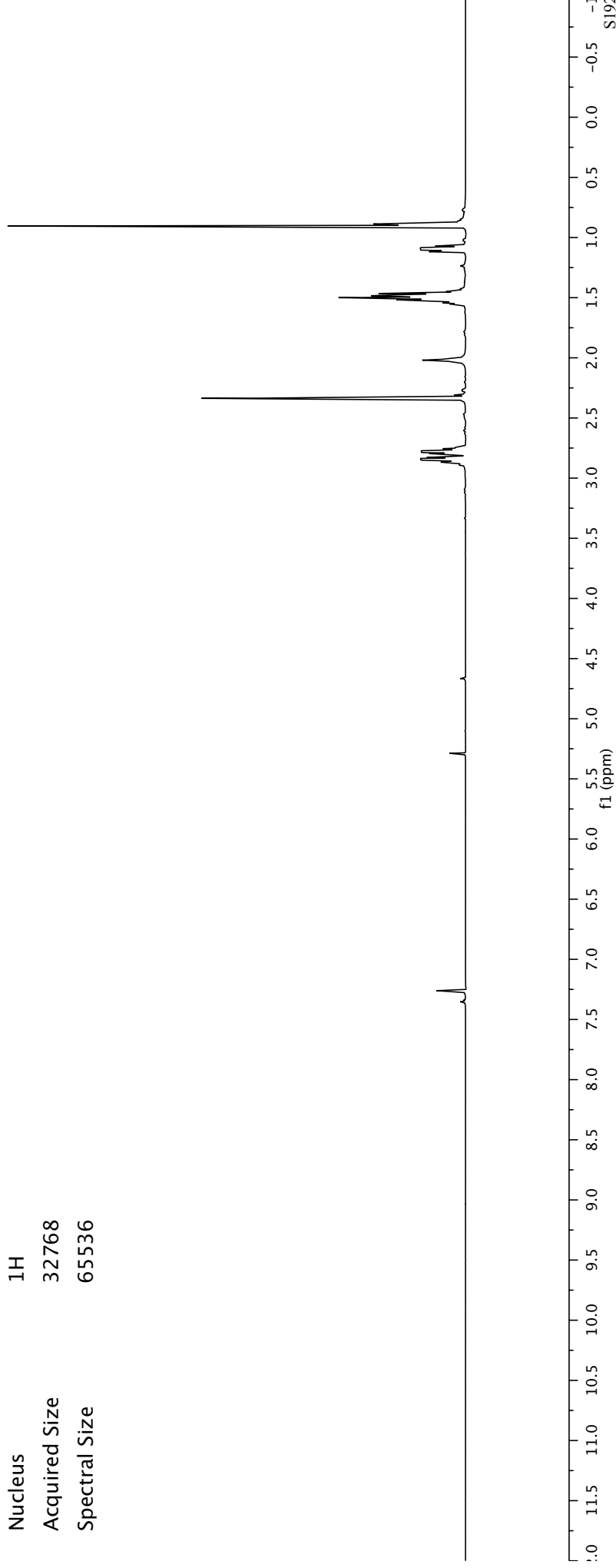
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Number of Scans	16
Receiver Gain	56
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	499.43
Spectral Width	8000.0
Lowest Frequency	-1509.2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

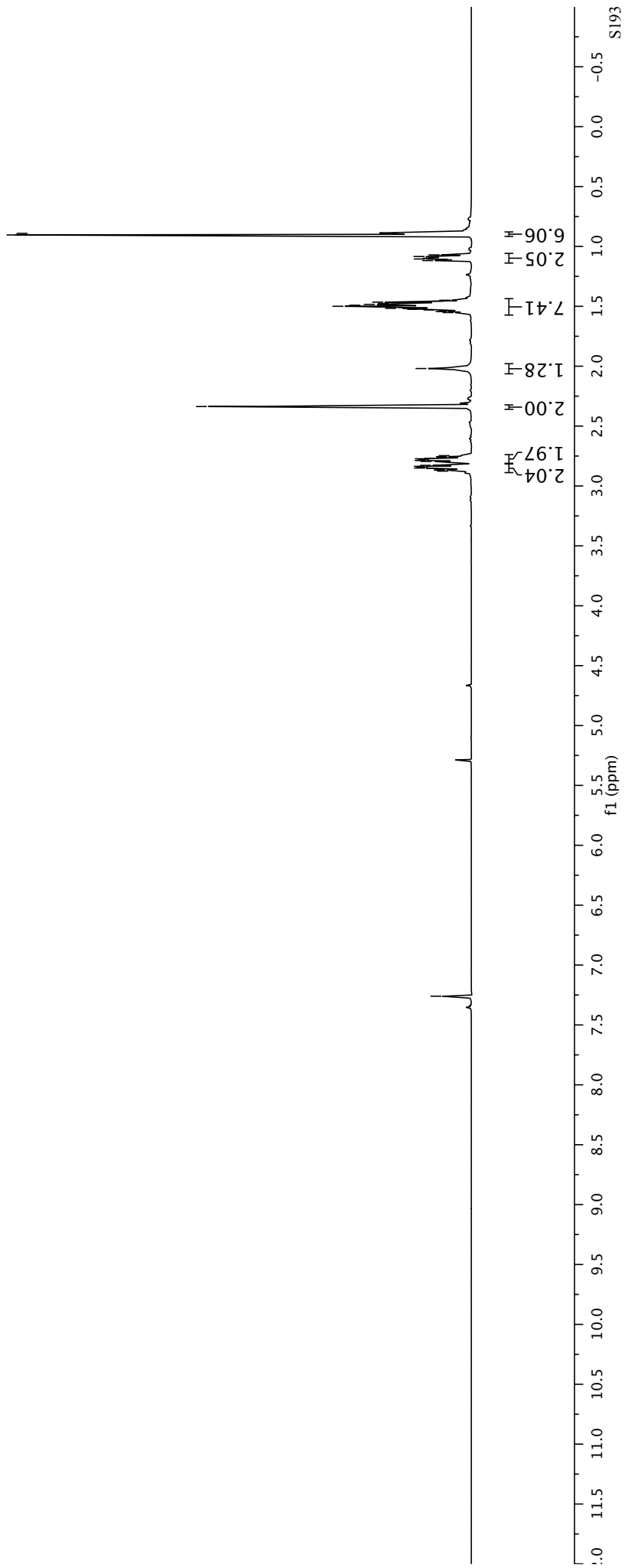
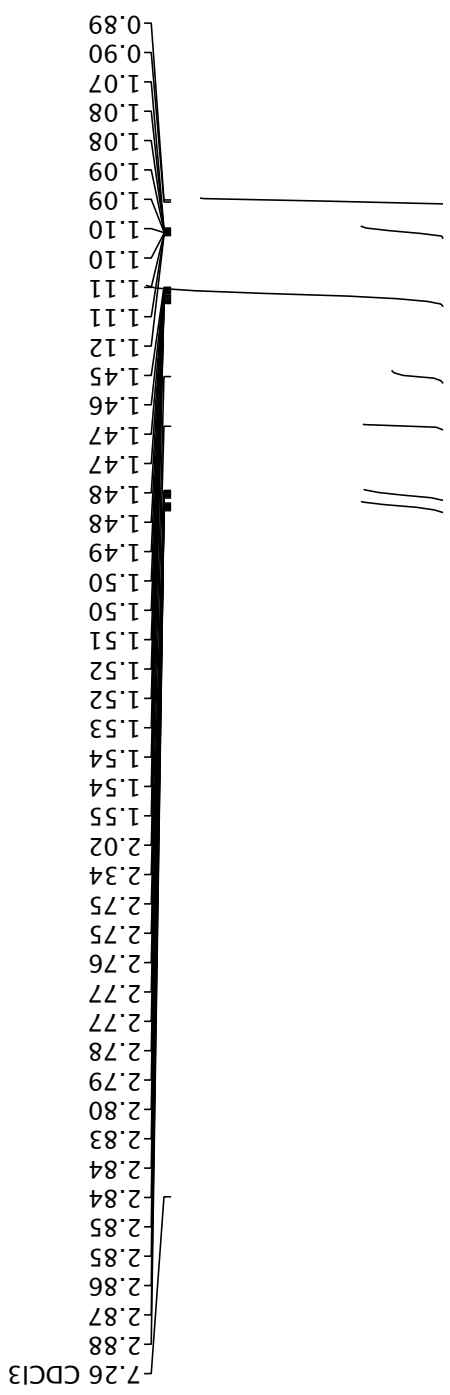
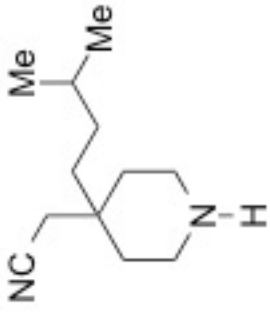


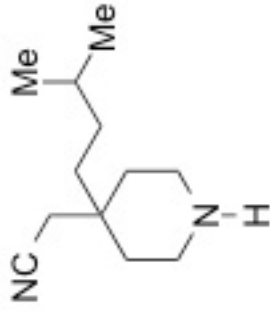




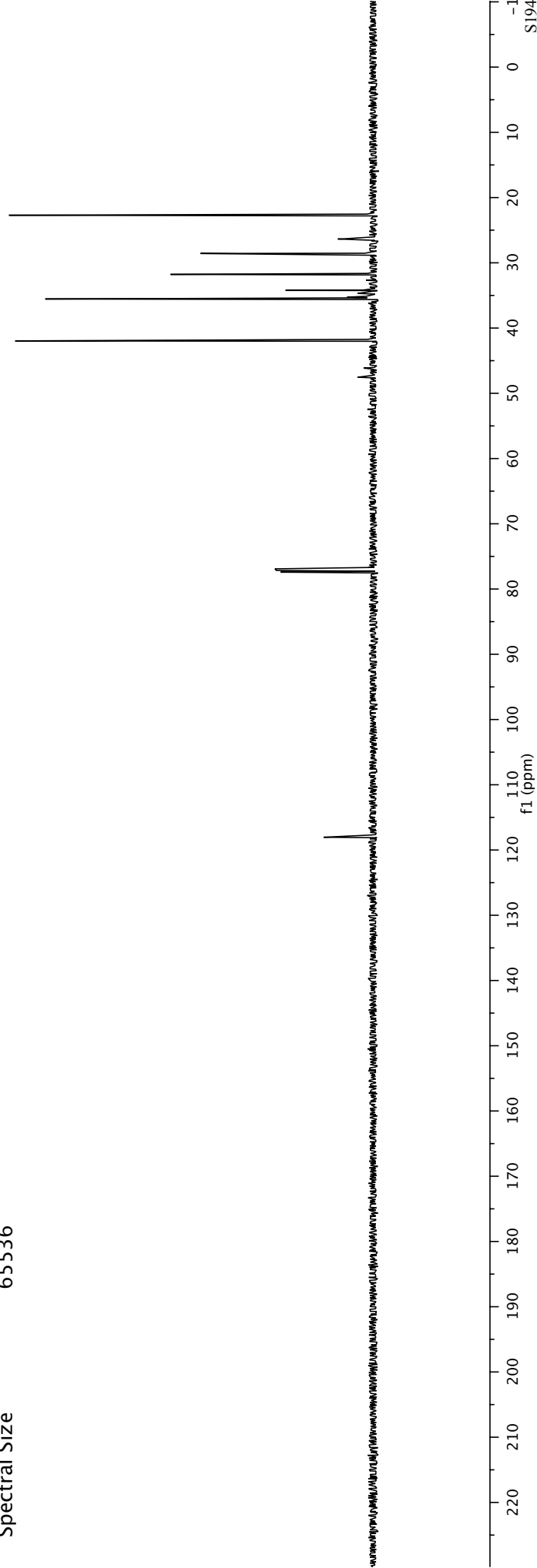
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	8
Receiver Gain	41
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.69
Spectral Width	7024.9
Lowest Frequency	-1021.9
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

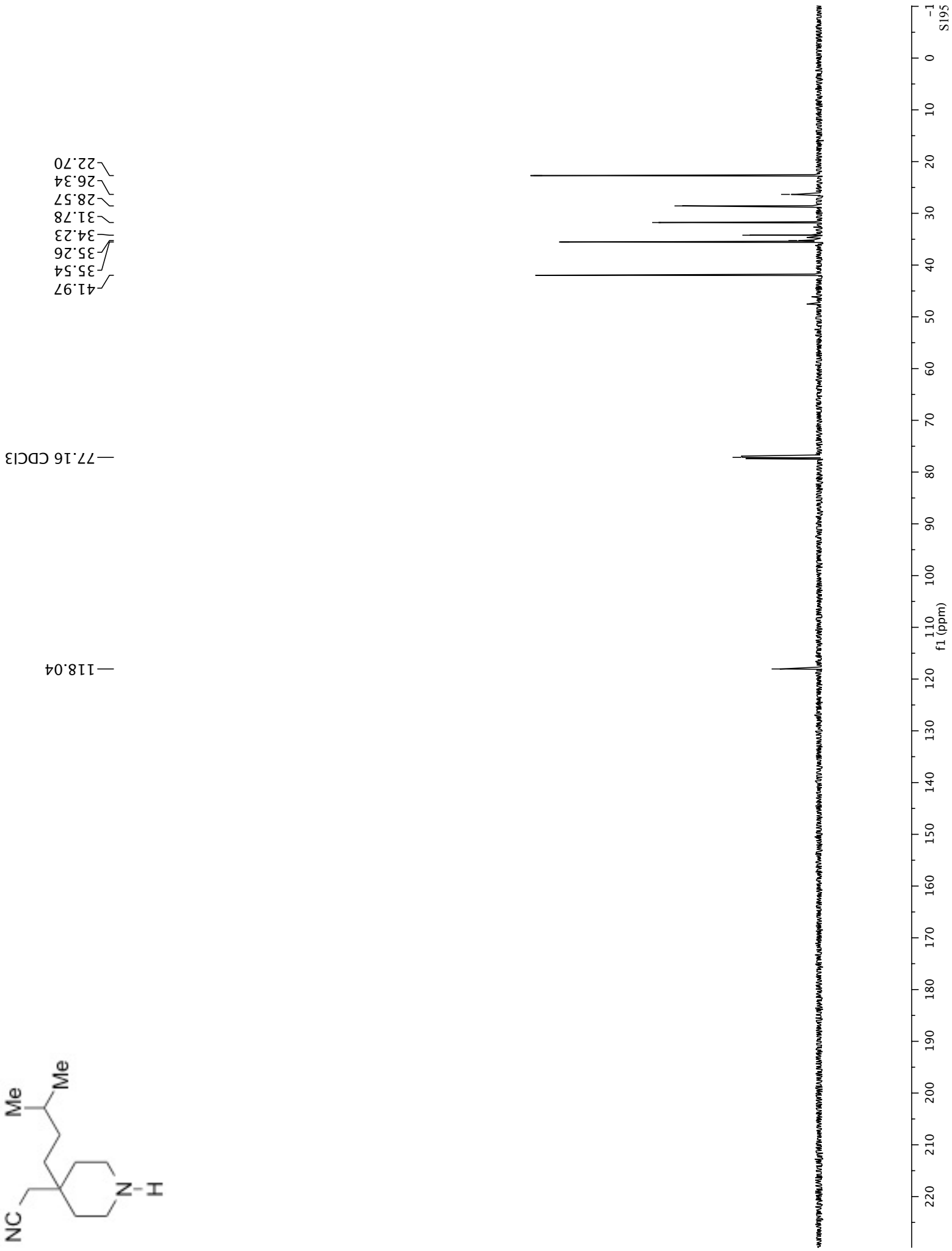
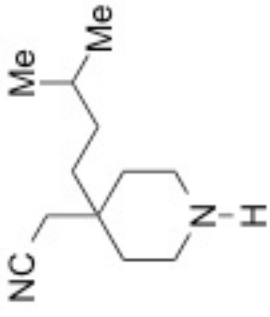


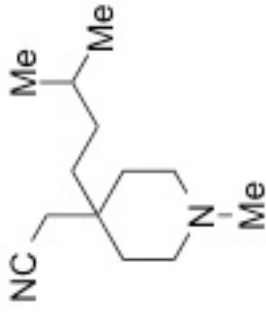




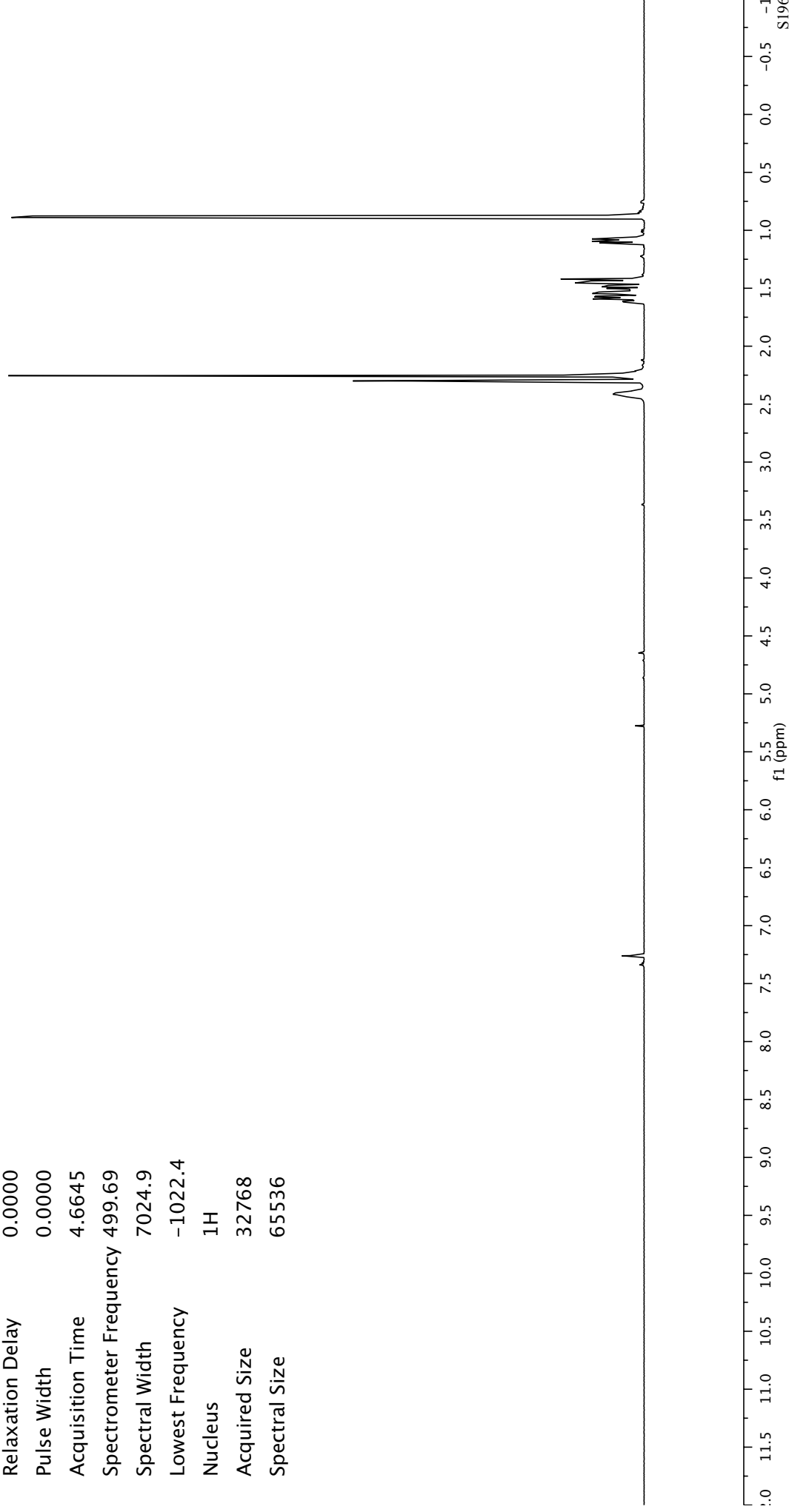
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	128
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1277.6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

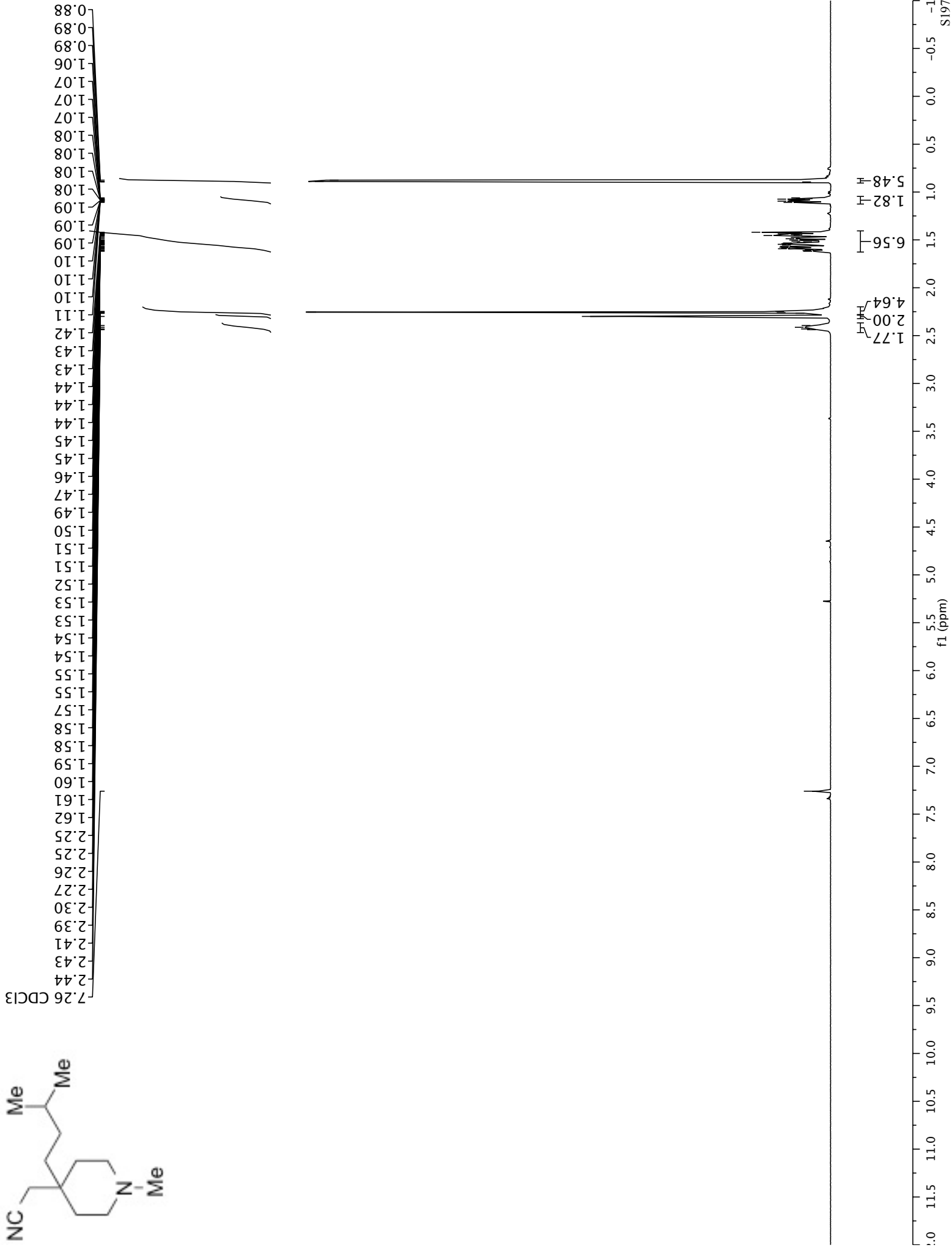
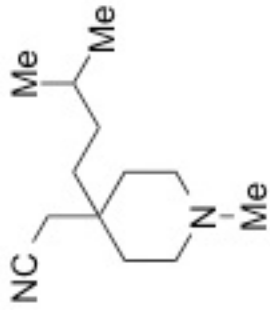


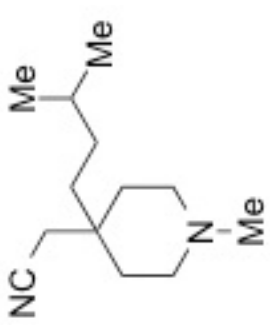




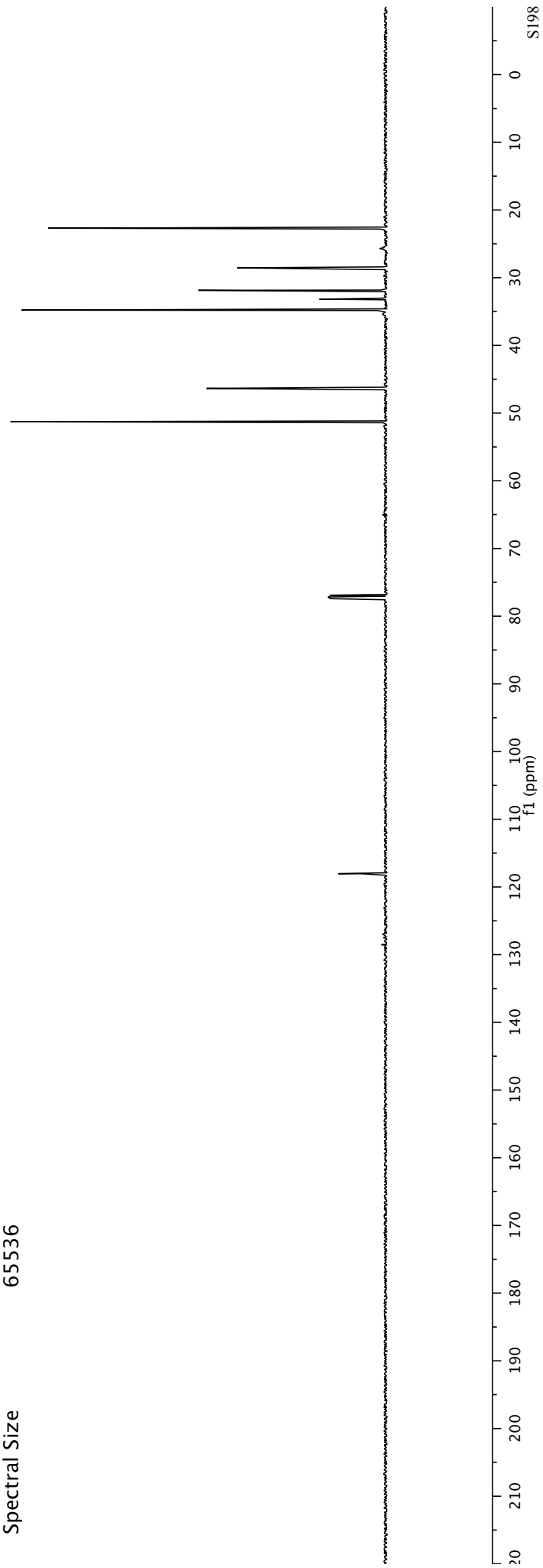
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	8
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.69
Spectral Width	7024.9
Lowest Frequency	-1022.4
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

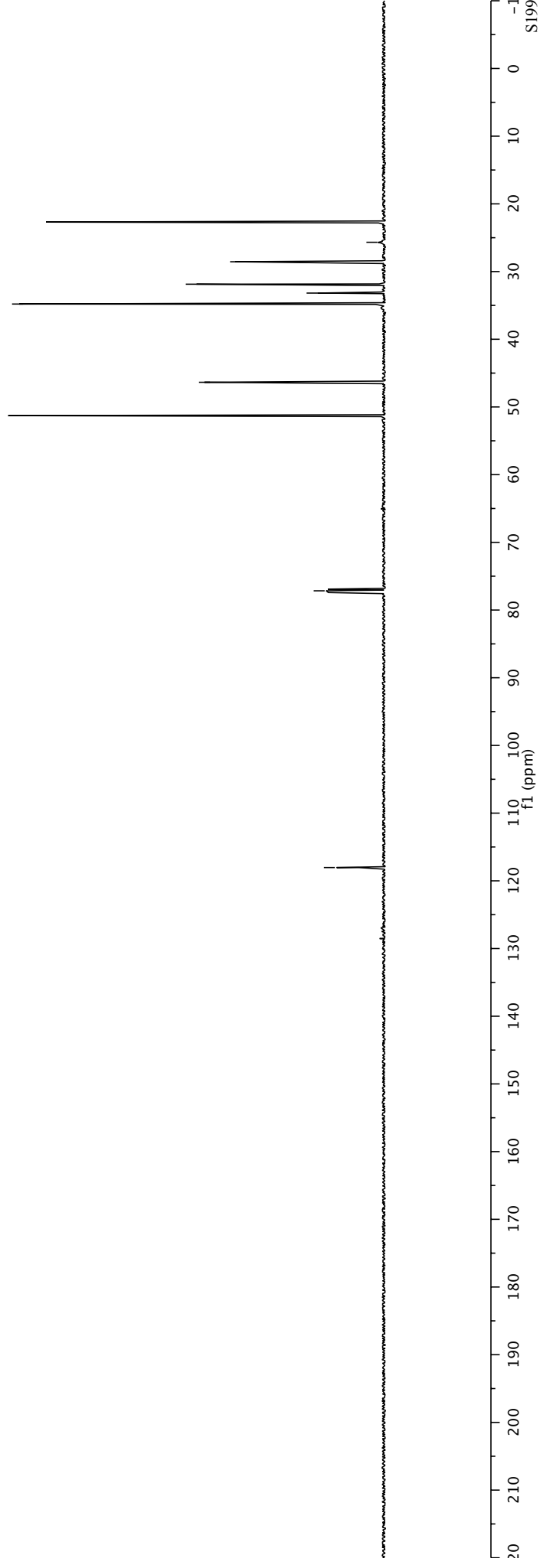
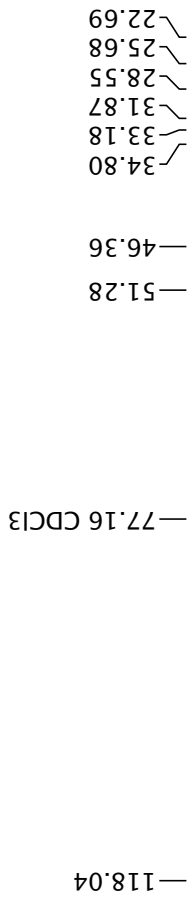
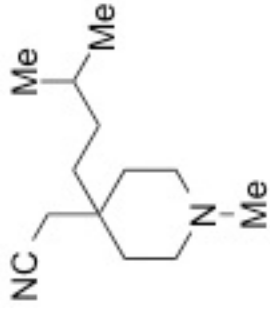


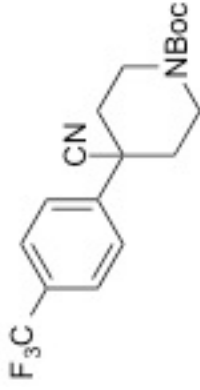




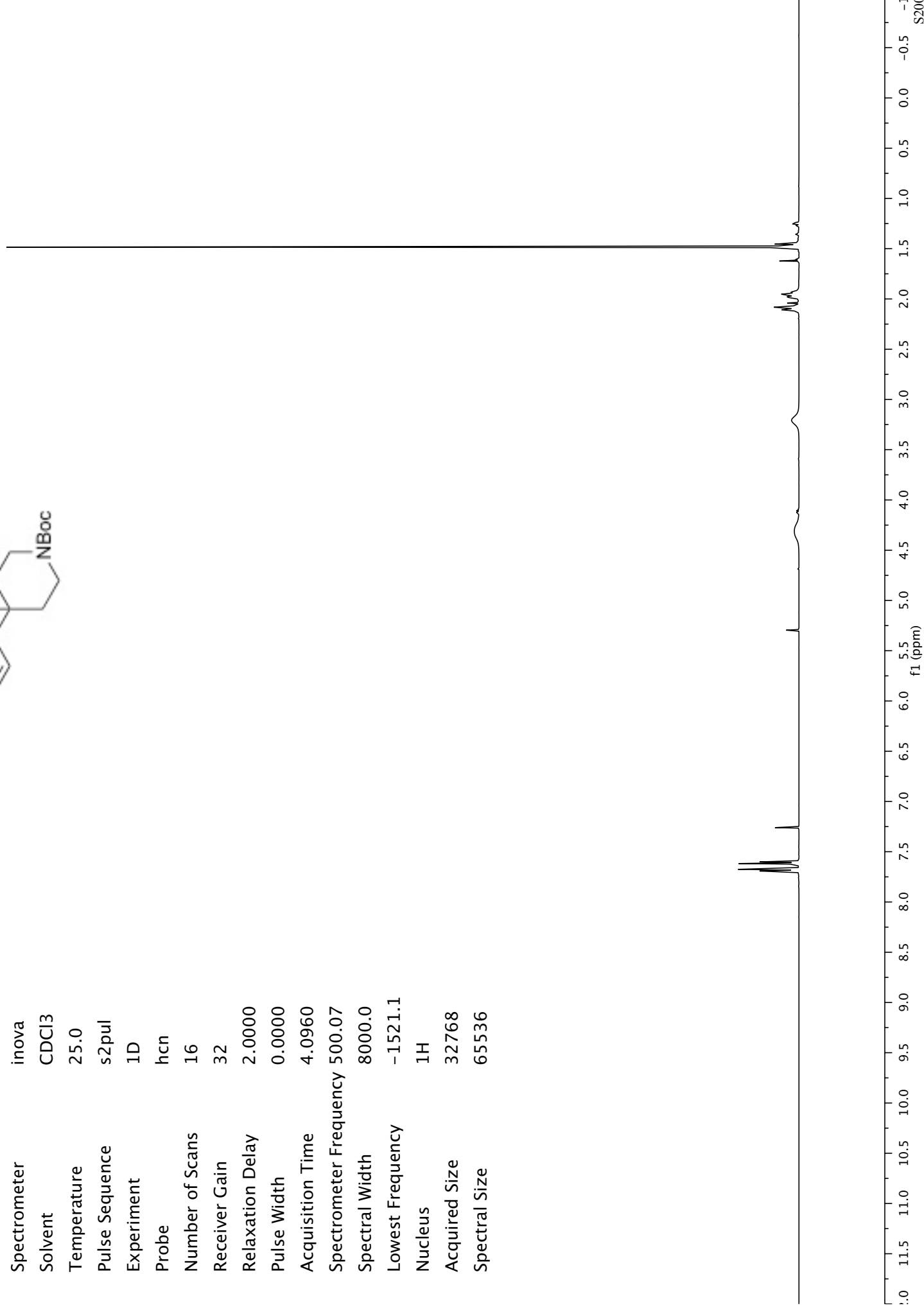
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	432
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1278.8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

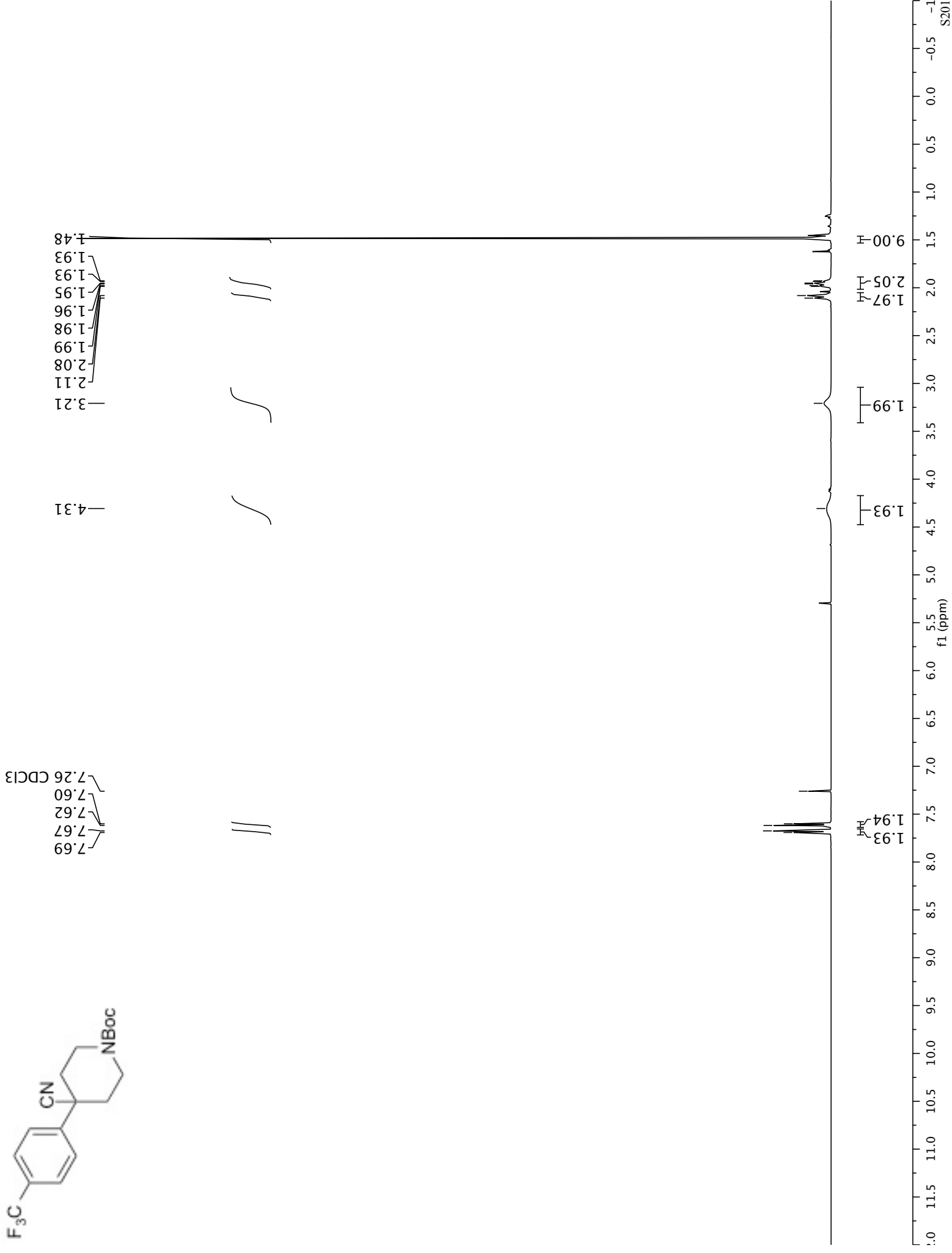
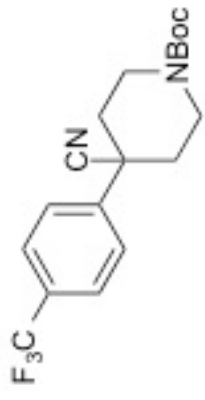


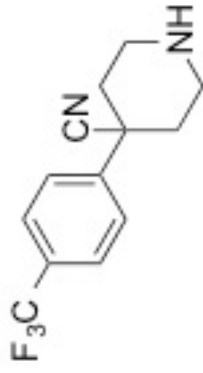




Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	32
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

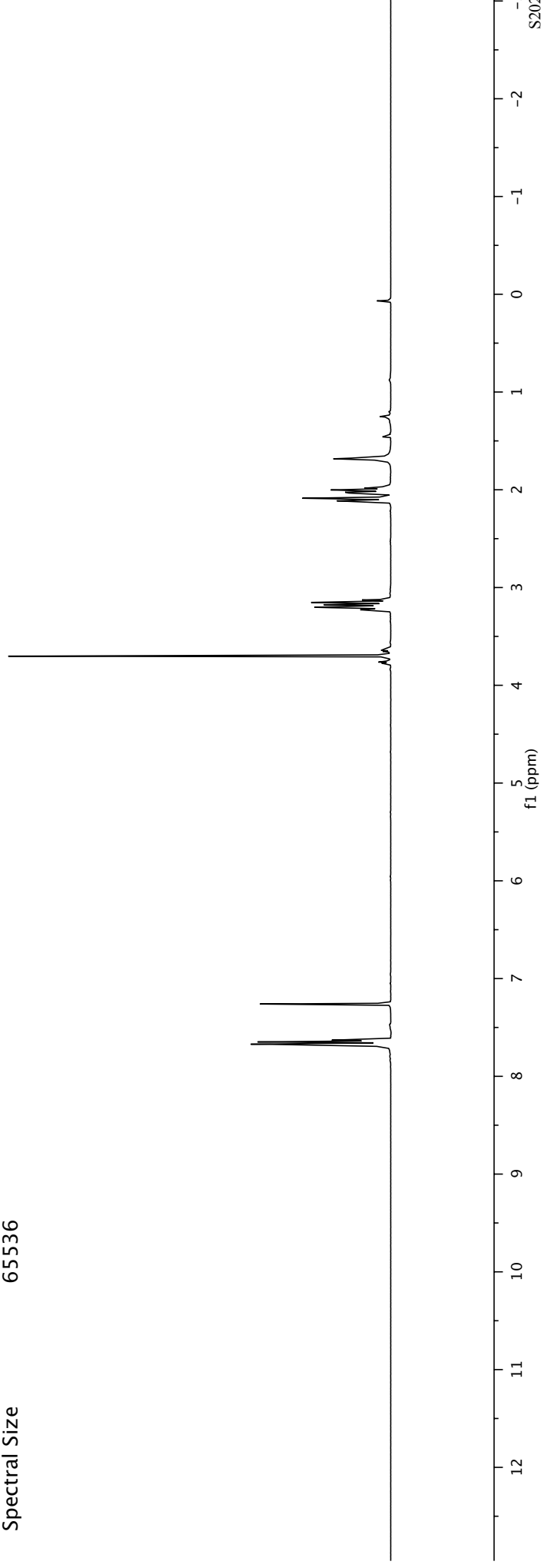


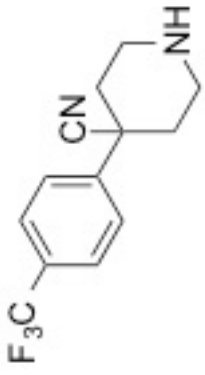




Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	42
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1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

1,4-dioxane

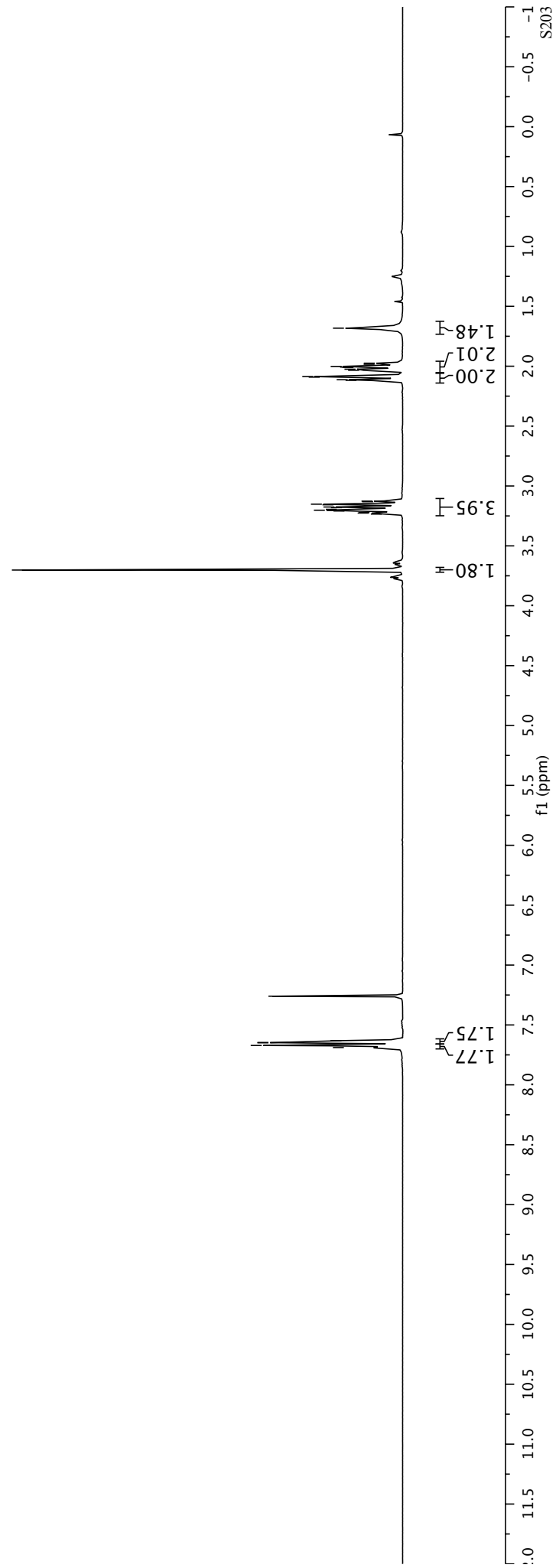


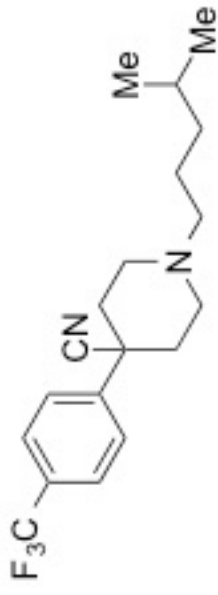


7.69
7.67
7.65
7.65
7.63
7.26 CDCl₃

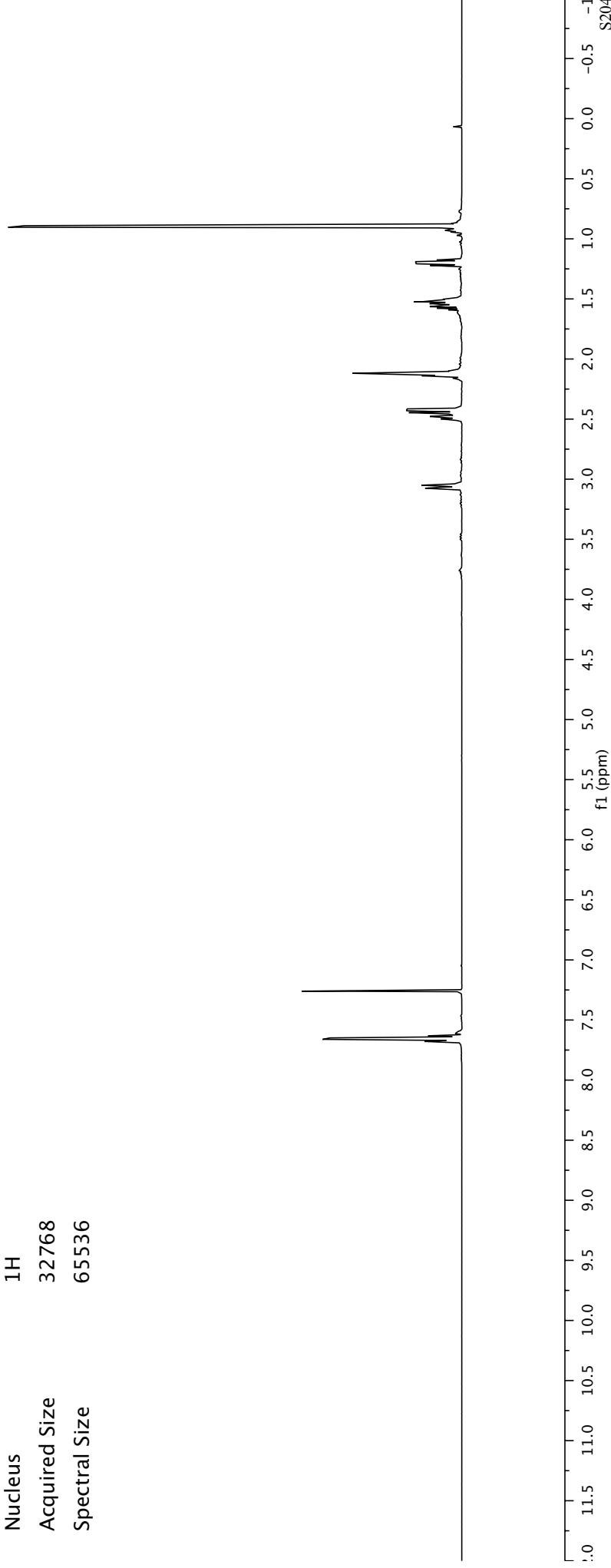
3.70
3.23
3.23
3.22
3.21
3.20
3.19
3.18
3.18
3.16
3.15
3.13
3.13
2.12
2.11
2.09
2.09
2.03
2.03
2.01
2.01
2.00
1.98
1.97
1.68

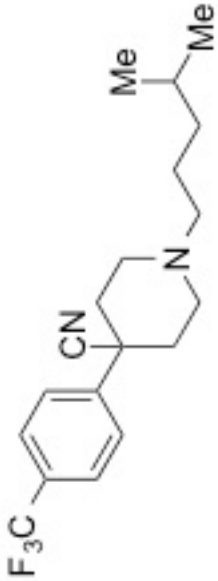
1,4-dioxane



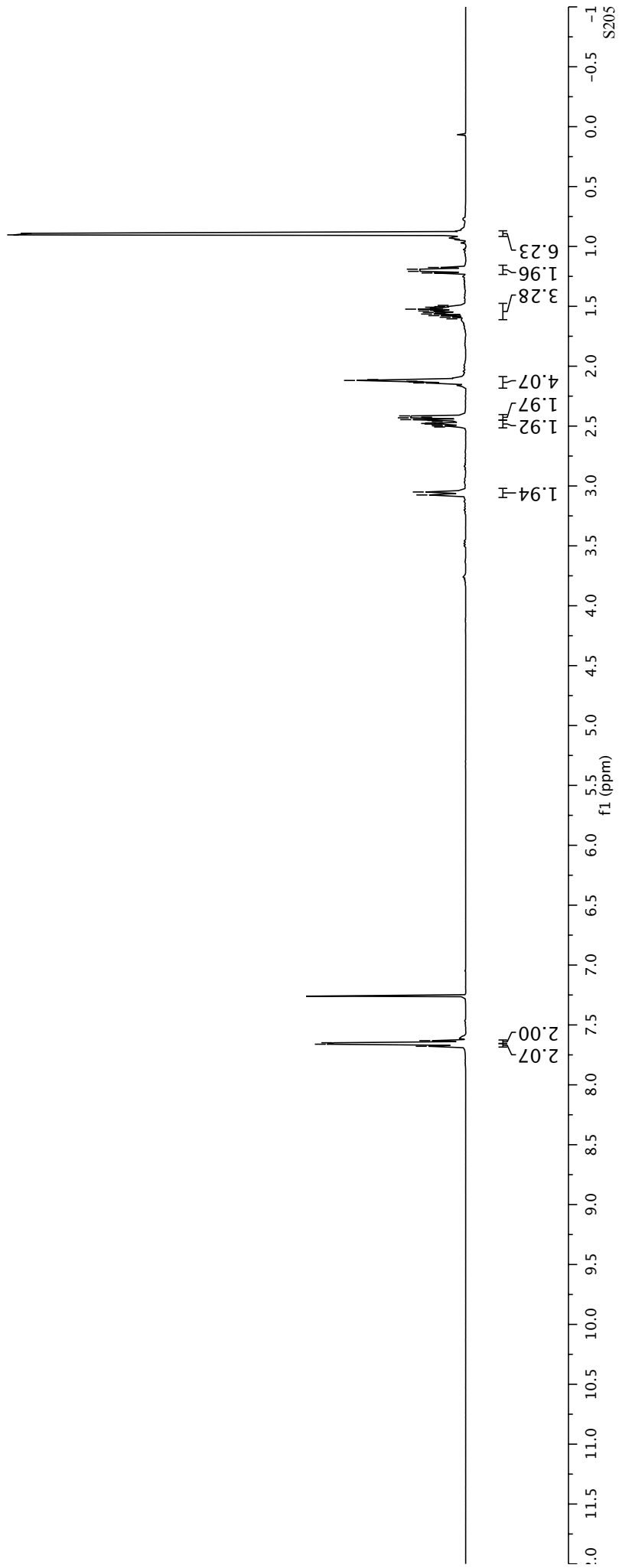
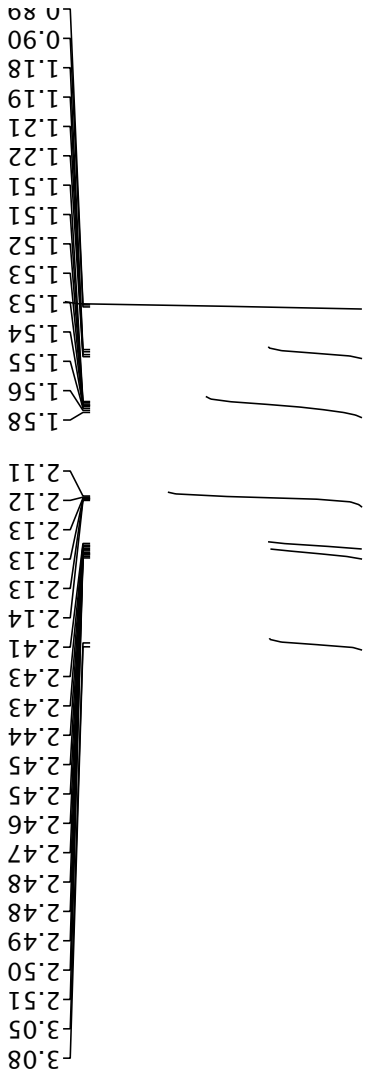


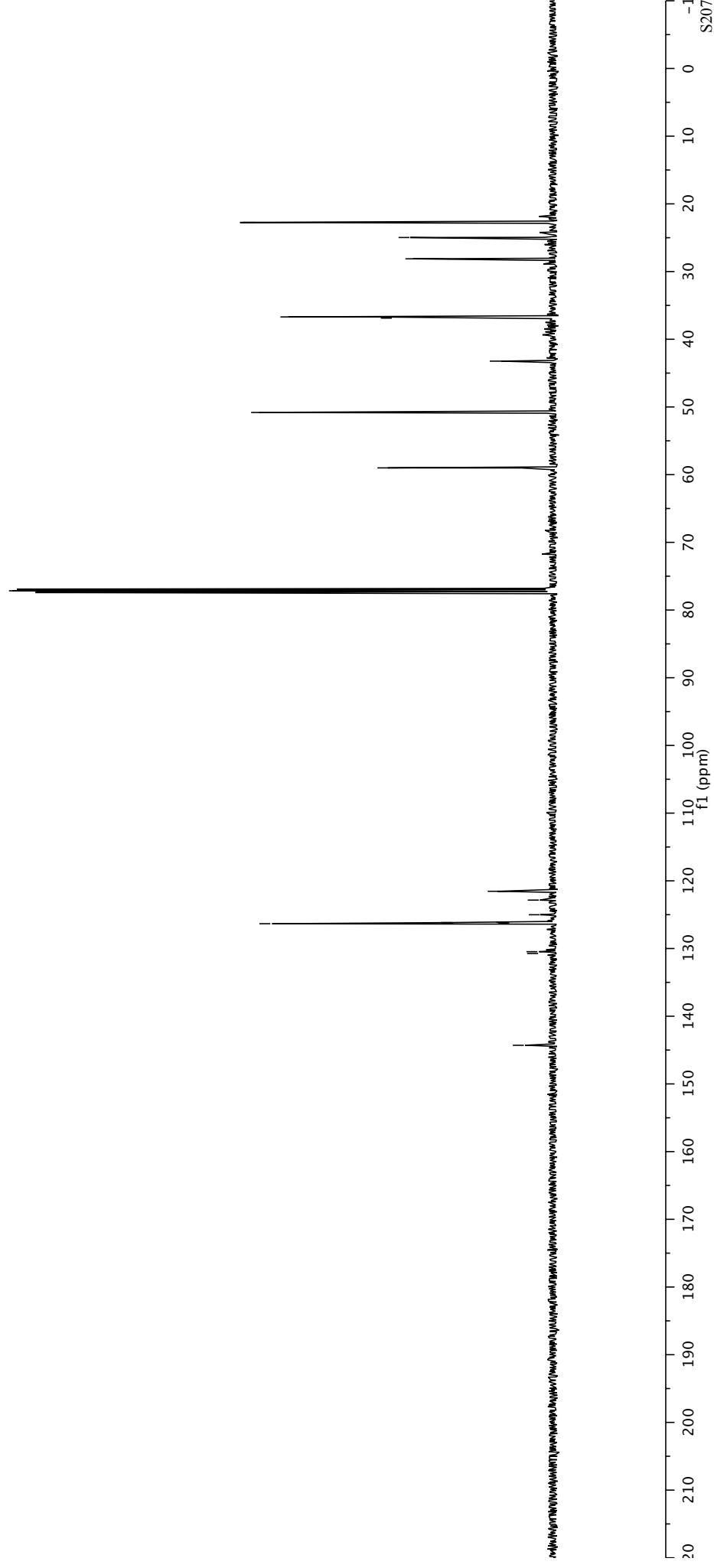
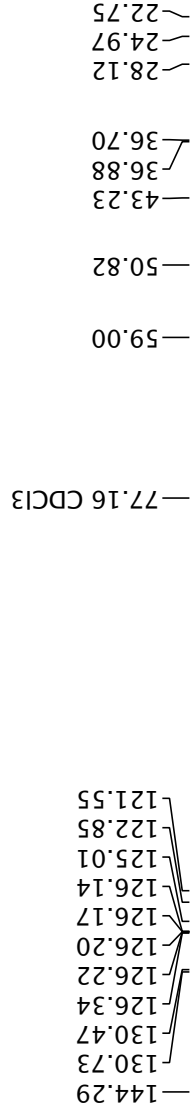
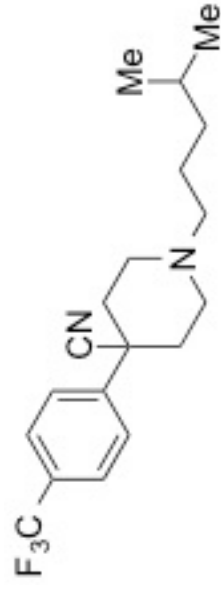
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	32
Relaxation Delay	15.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.6
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

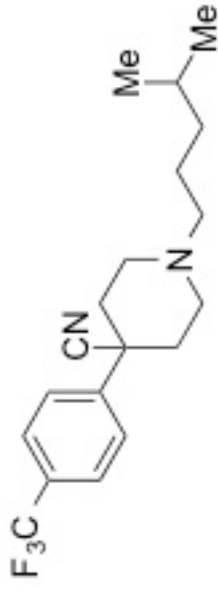




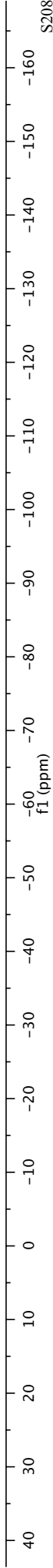
7.68
7.66
7.65
7.63
7.26 CDCl₃

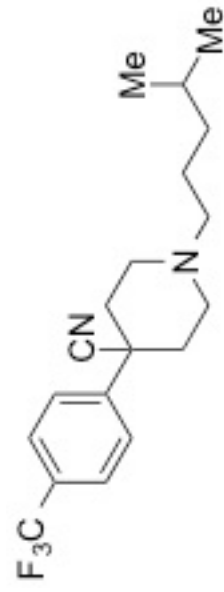




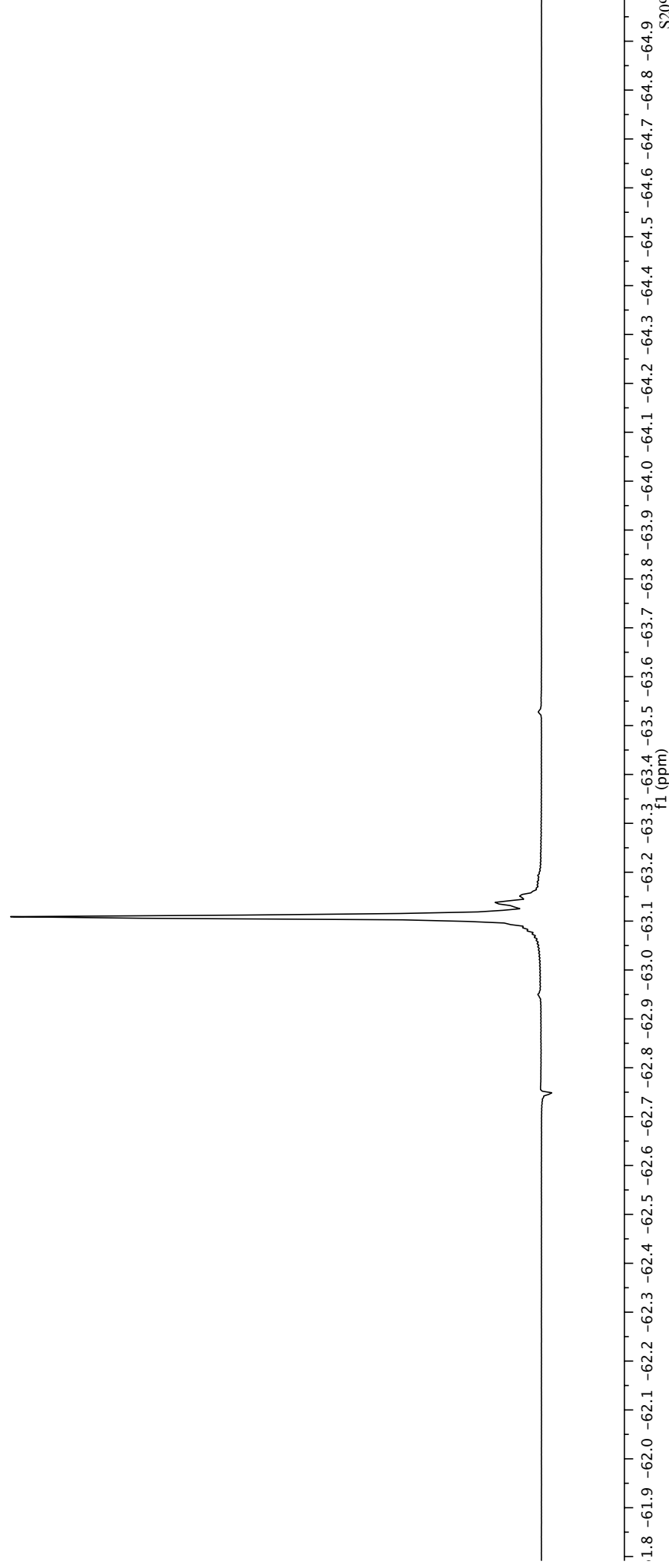


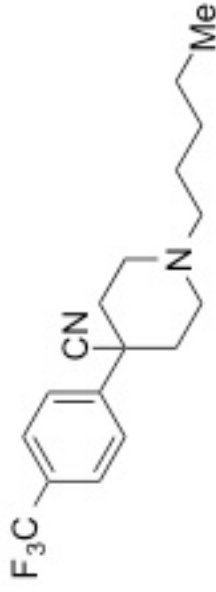
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	128
Receiver Gain	52
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency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



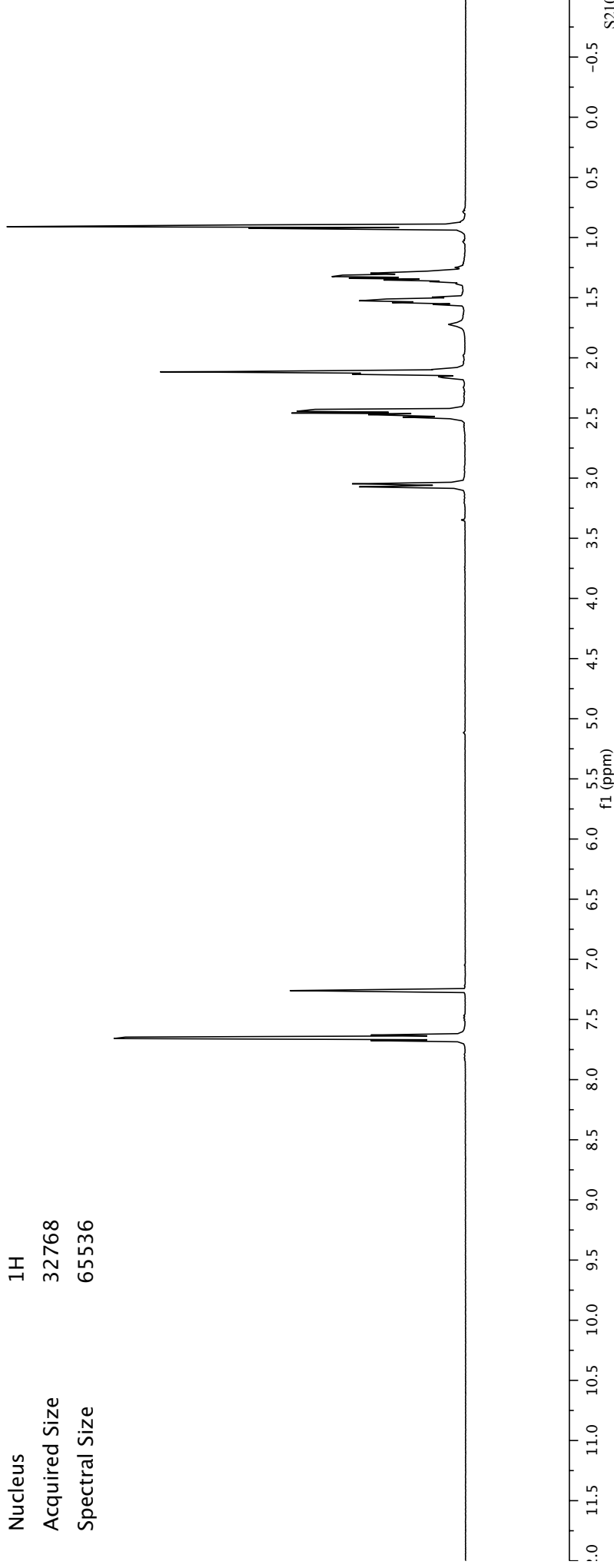


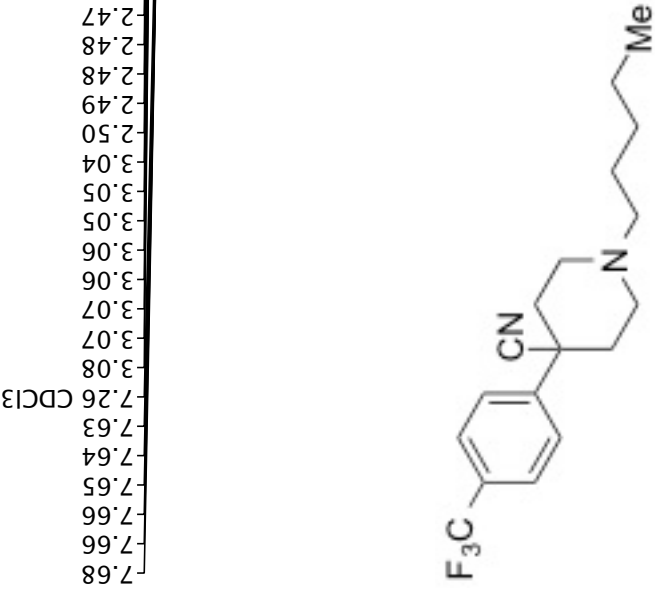
63.11



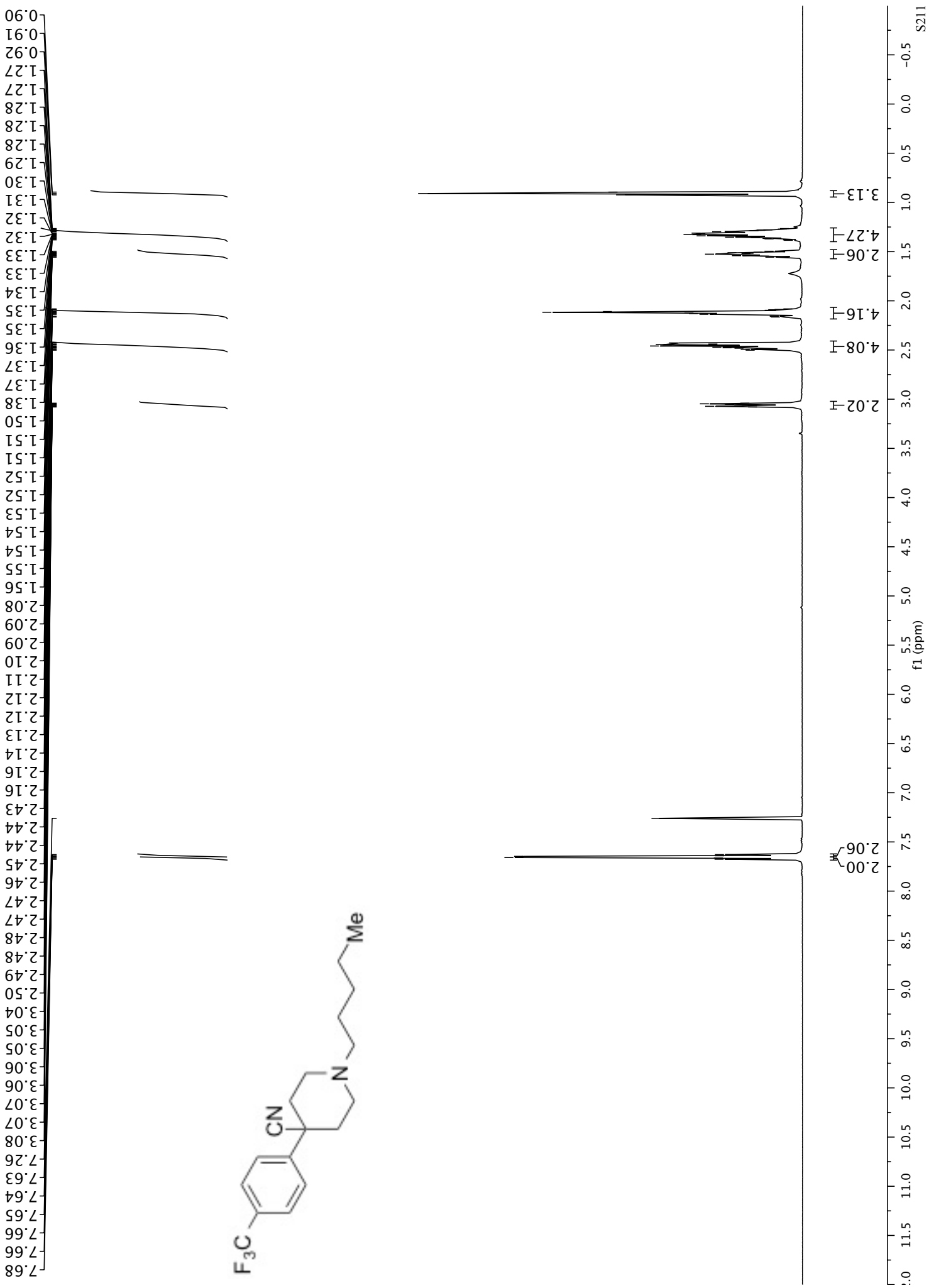


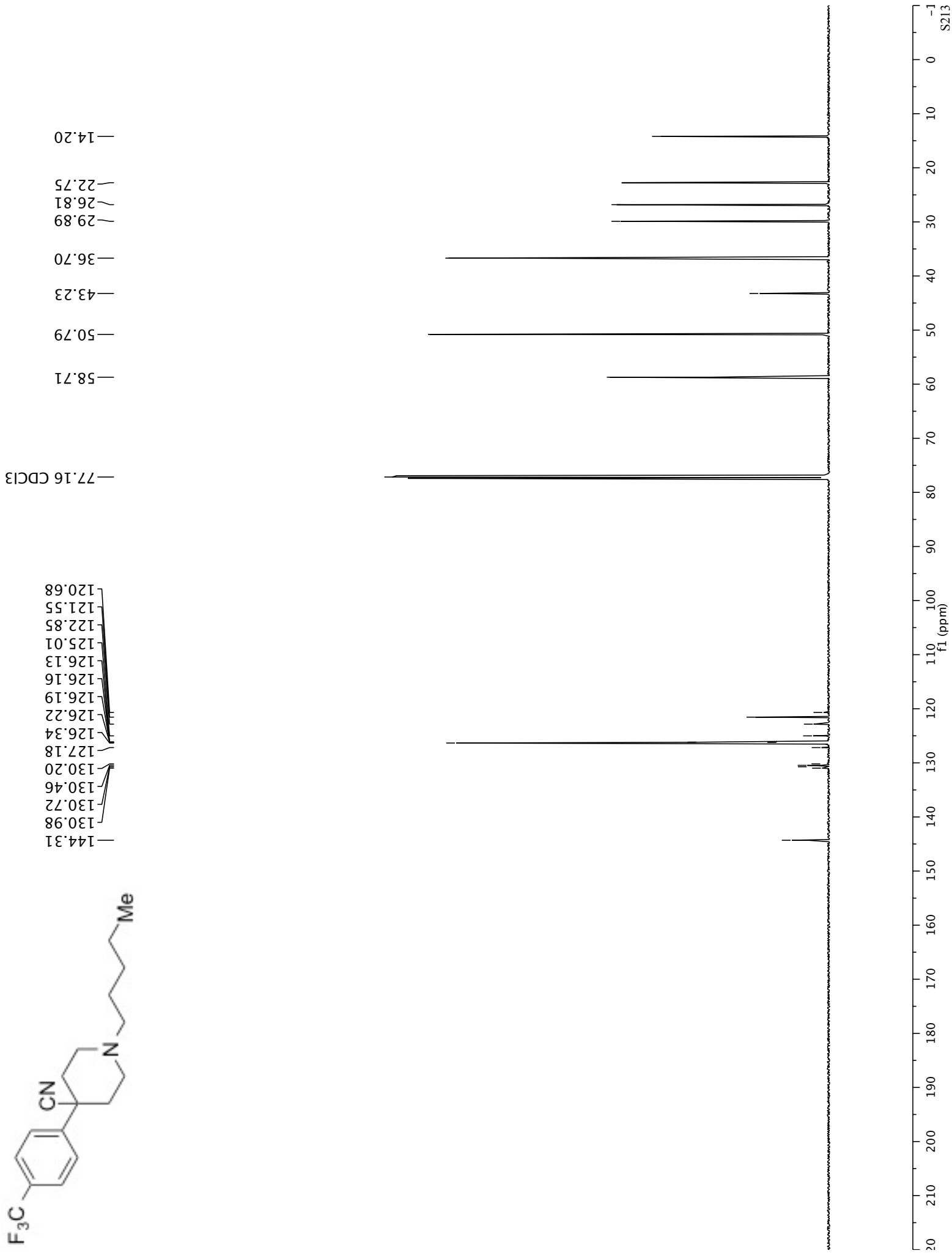
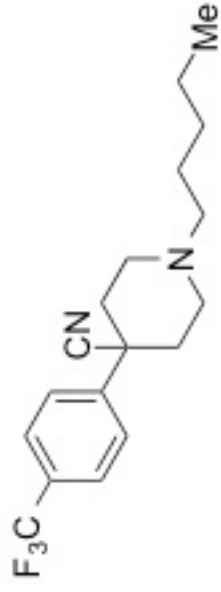
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	16
Receiver Gain	46
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.69
Spectral Width	7024.9
Lowest Frequency	-1021.9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

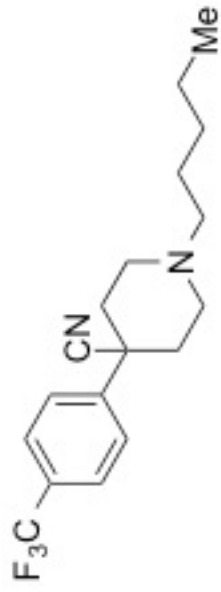




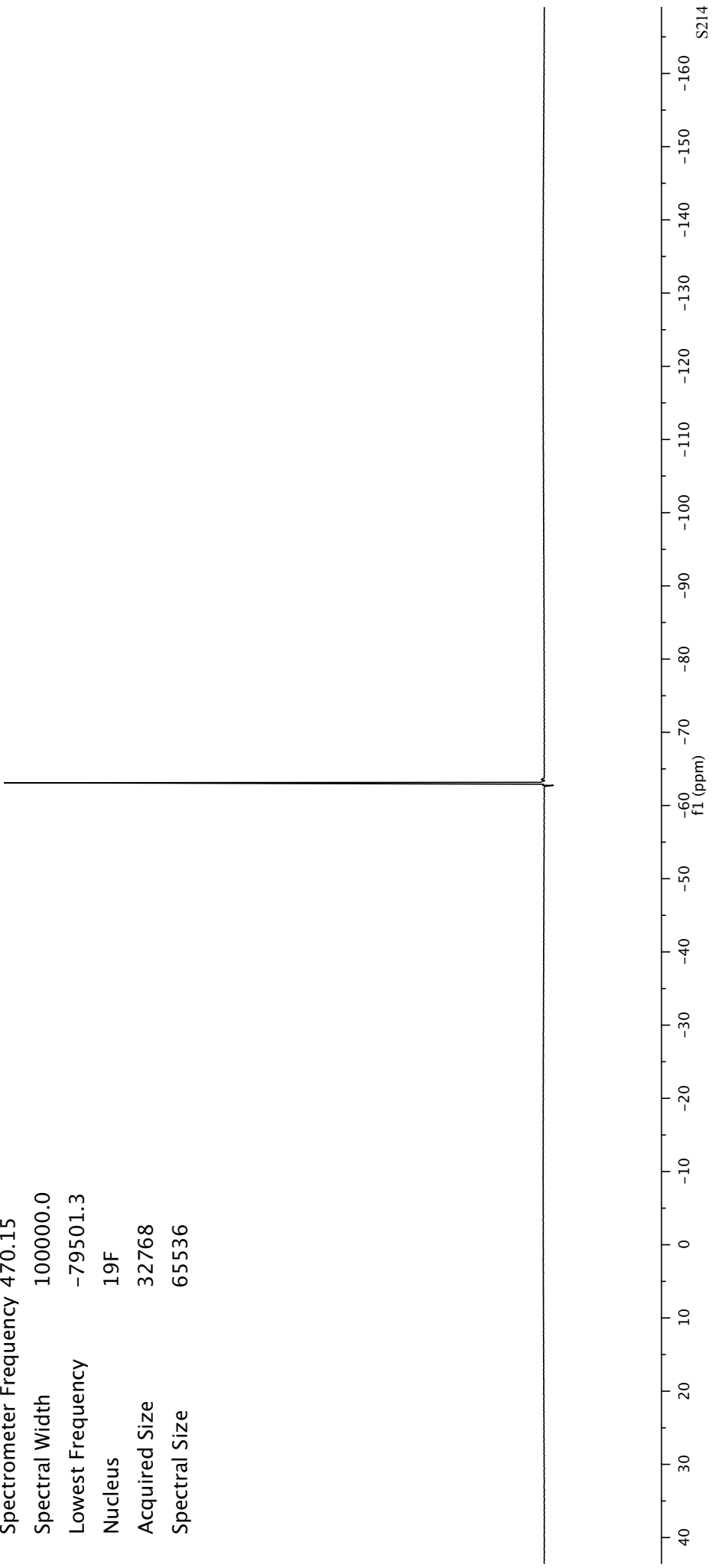
CDCl₃



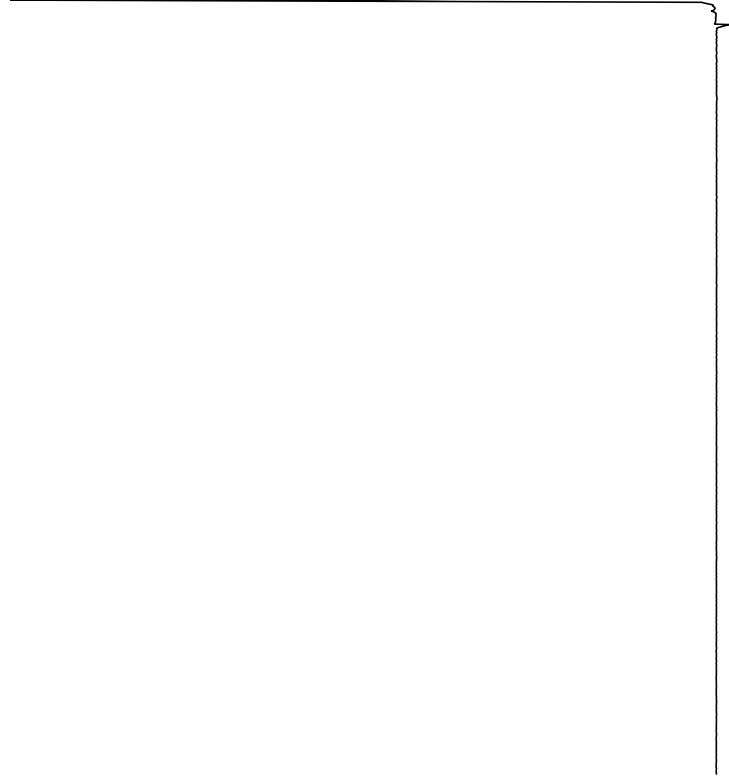
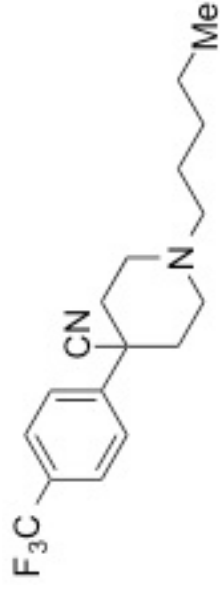


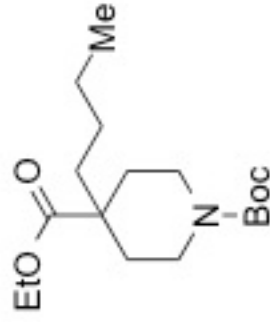


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	132
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency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

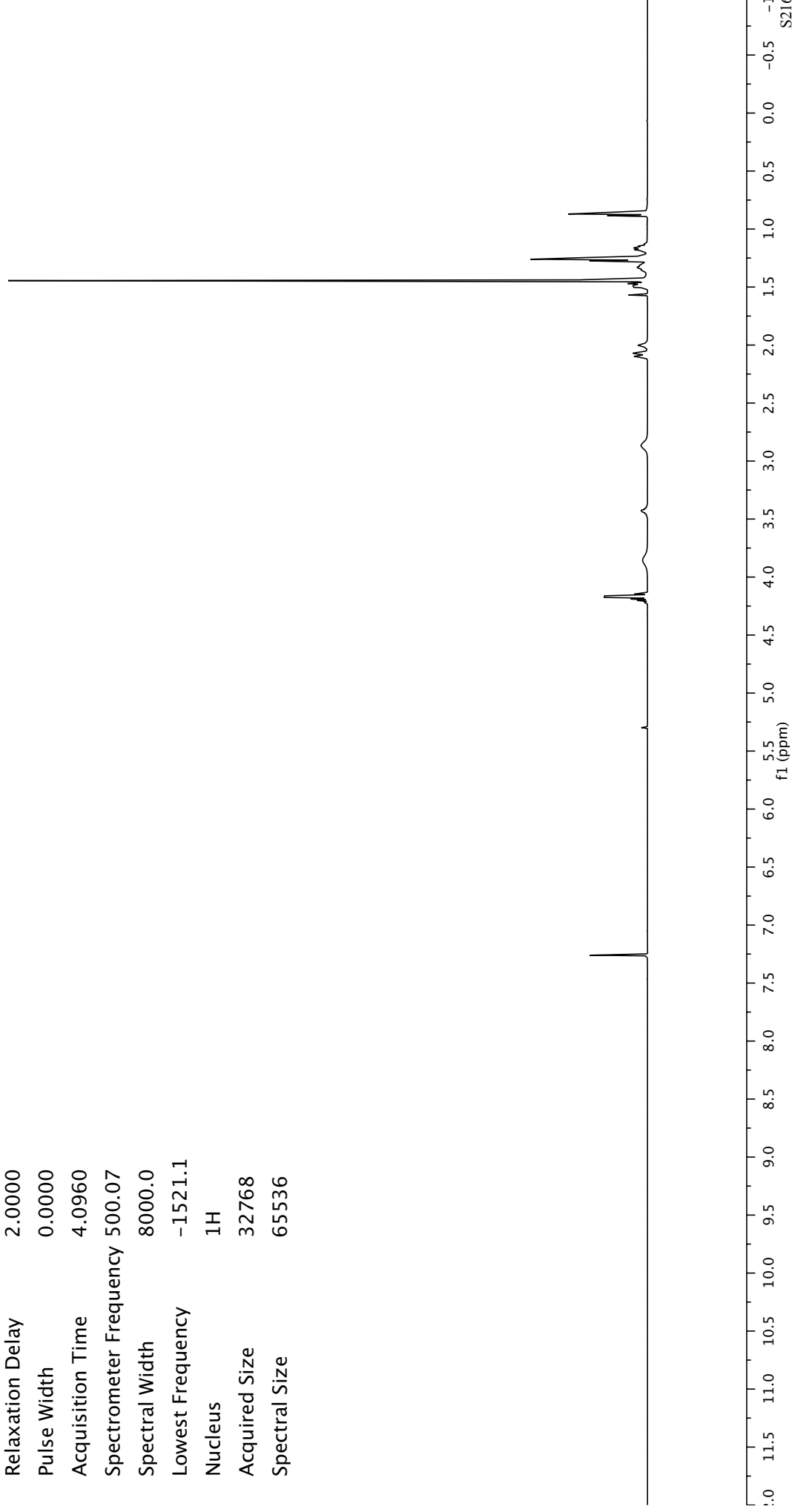


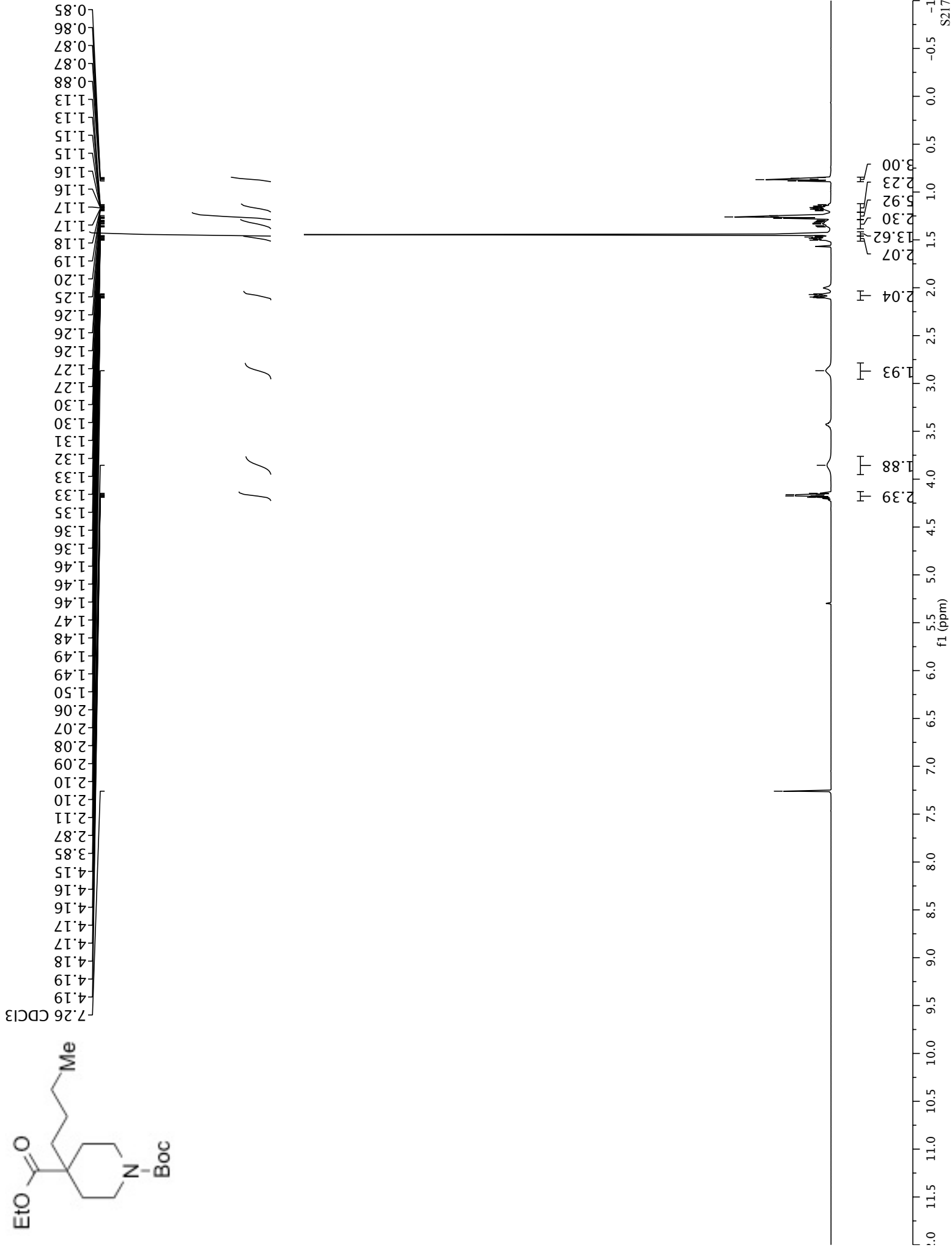
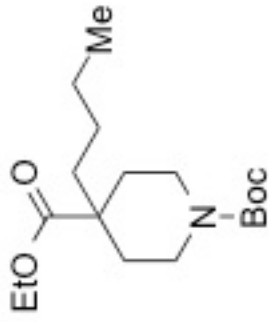
—63.11

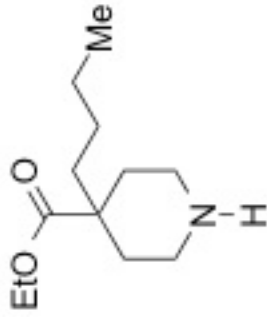




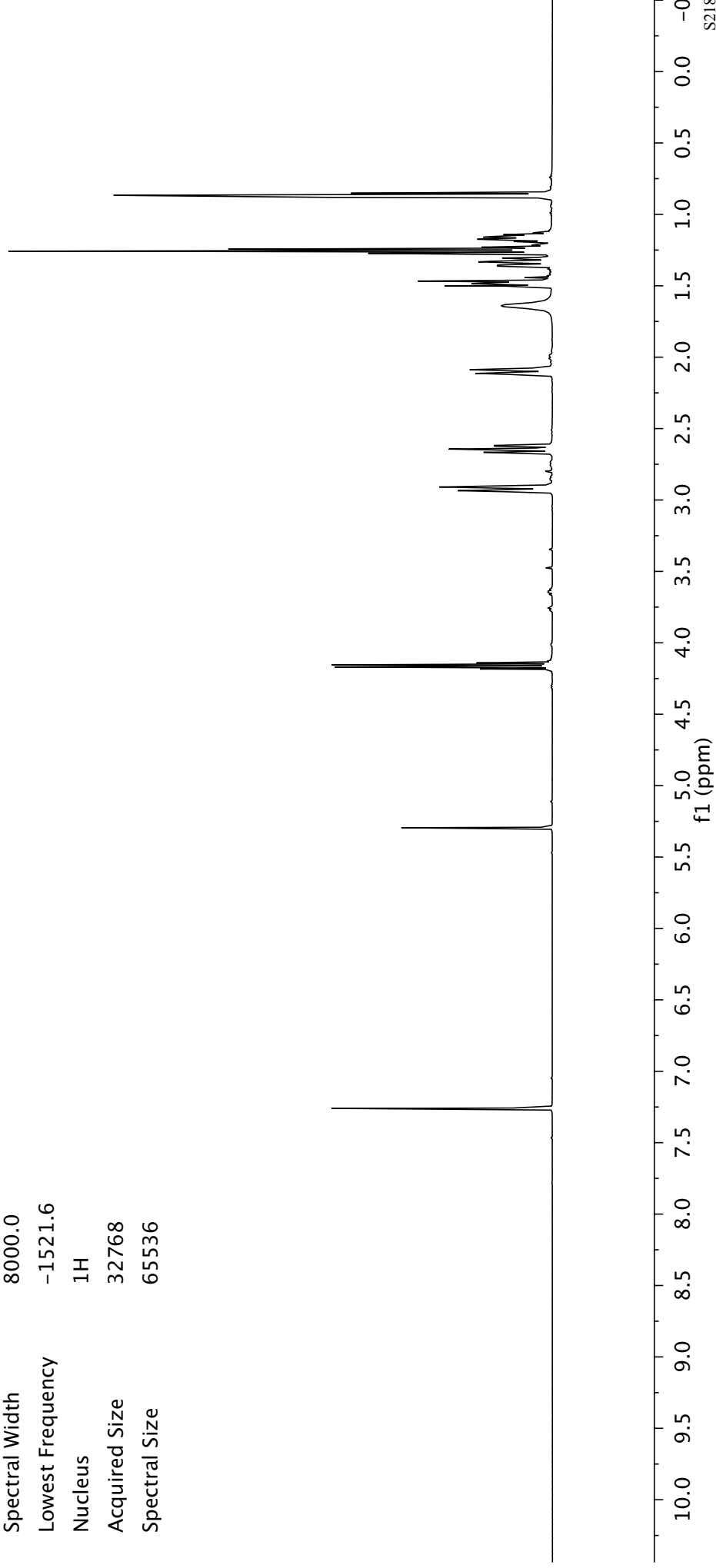
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	32
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1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

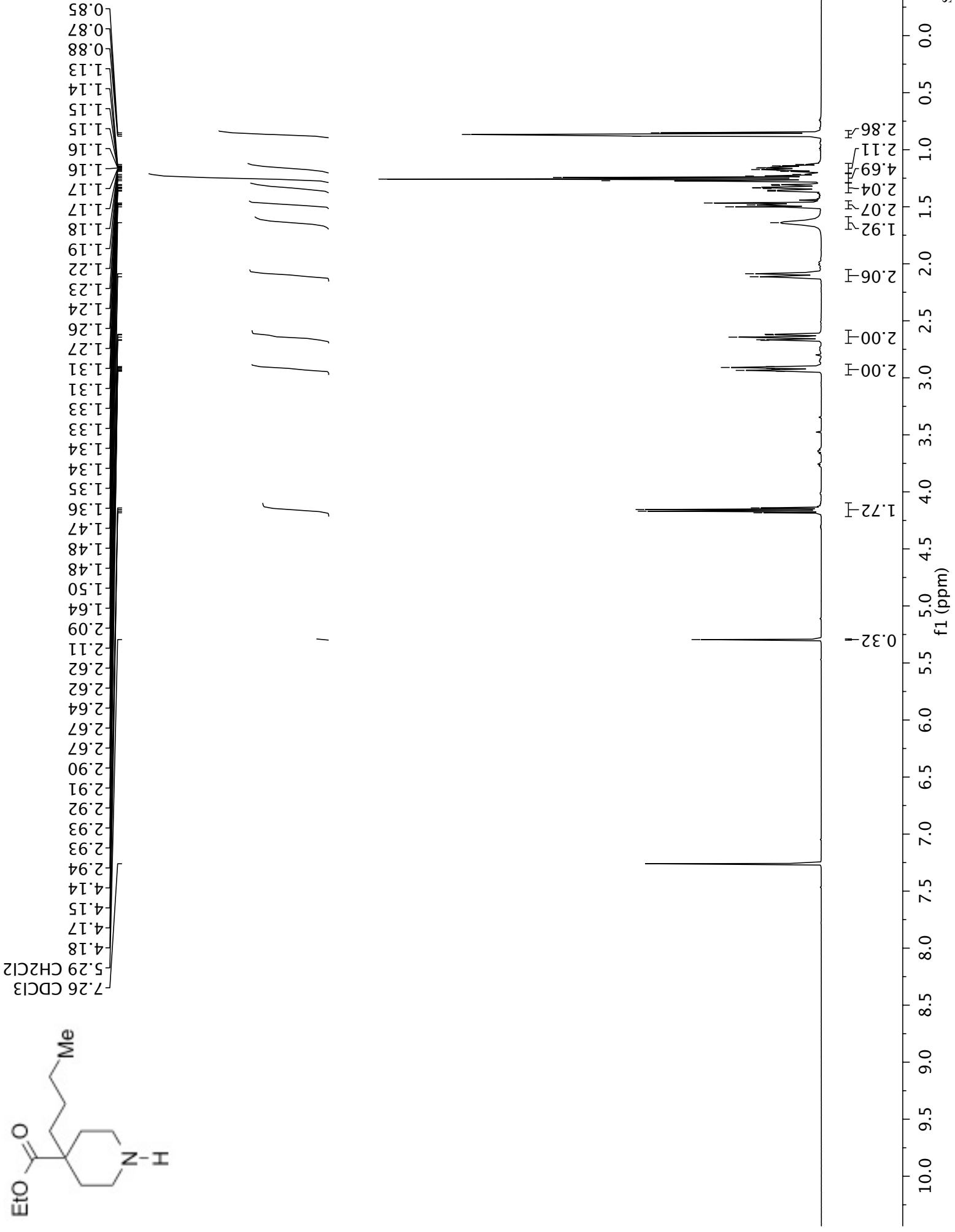
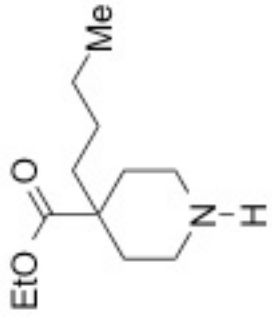


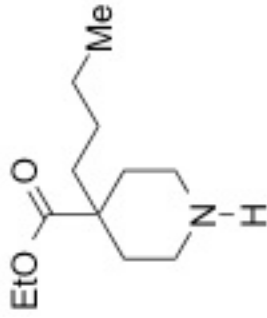




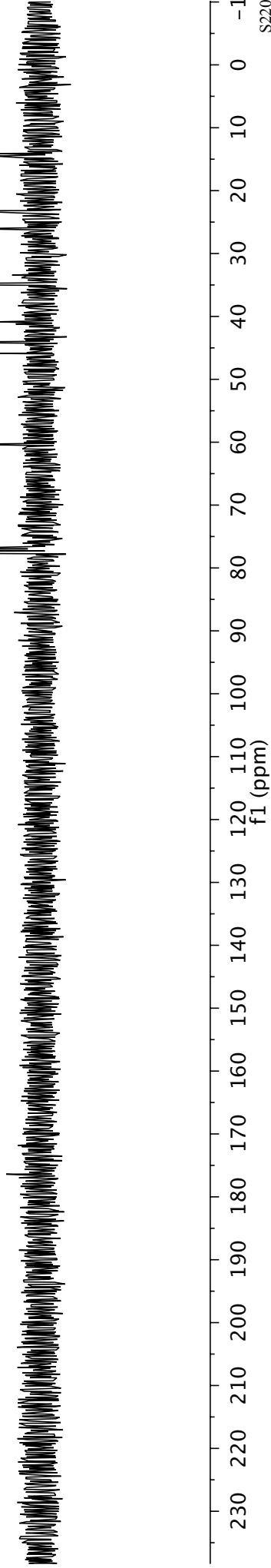
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	32
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.6
Nucleus	1H
Acquired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

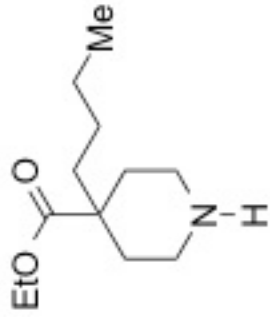






Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.3107
Spectrometer Frequency	100.58
Spectral Width	25000.0
Lowest Frequency	-1025.5
Nucleus	13C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

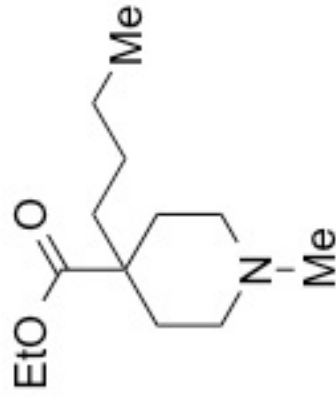
— 26.05

— 23.21

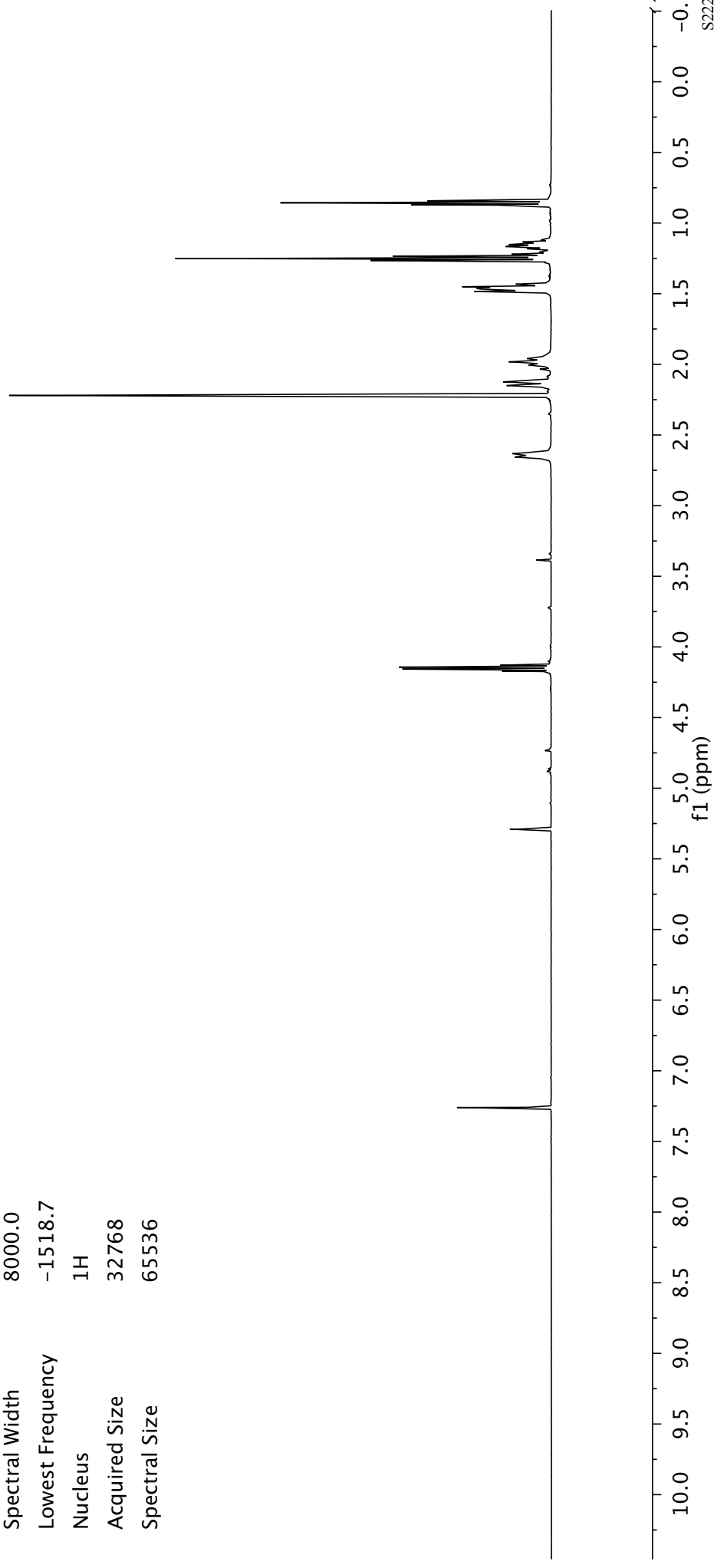
— 14.51

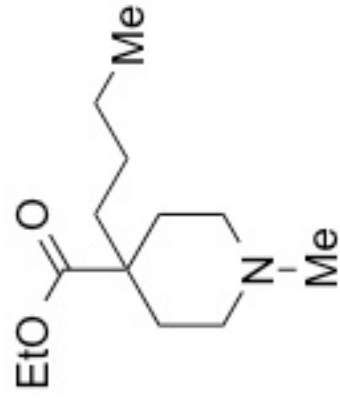
— 14.08





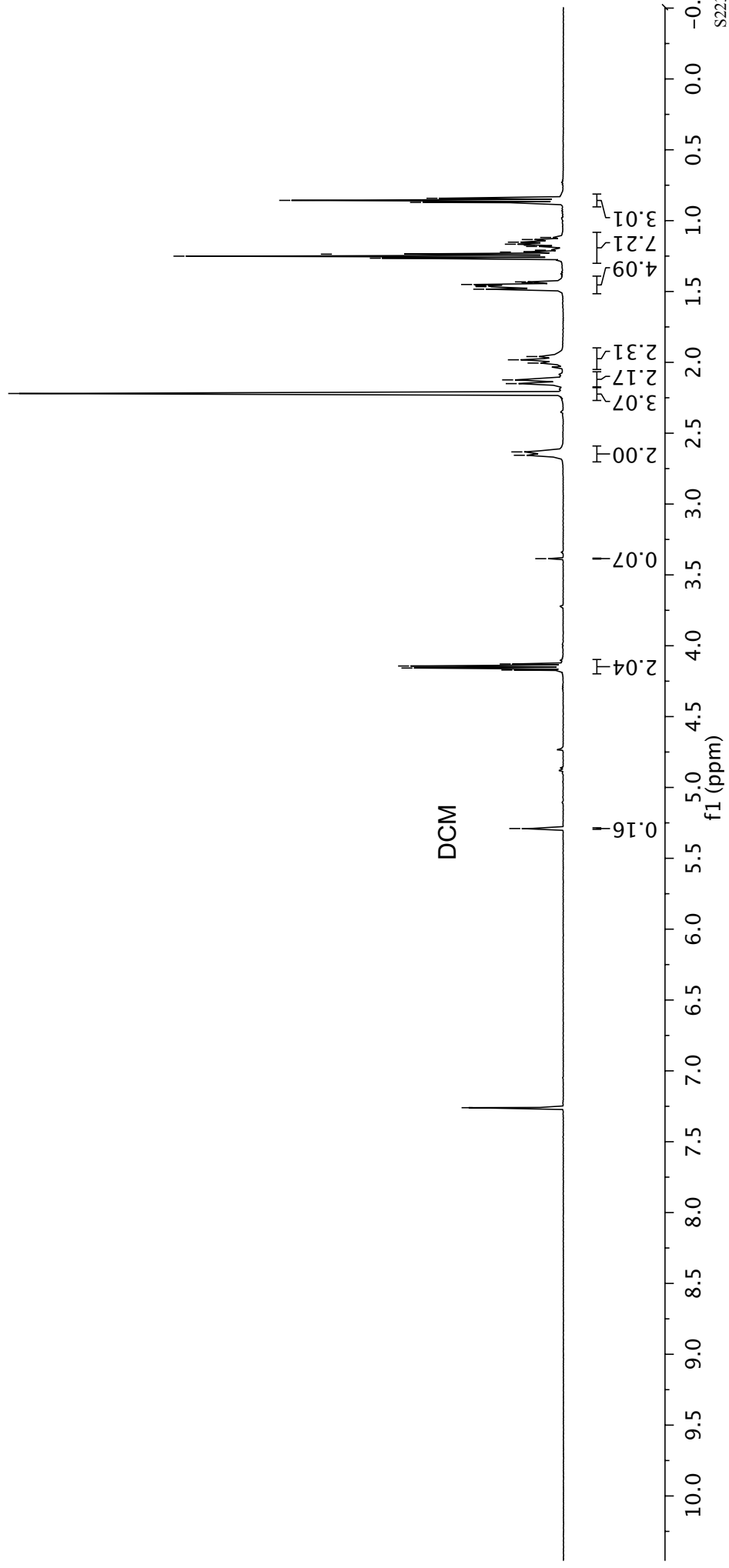
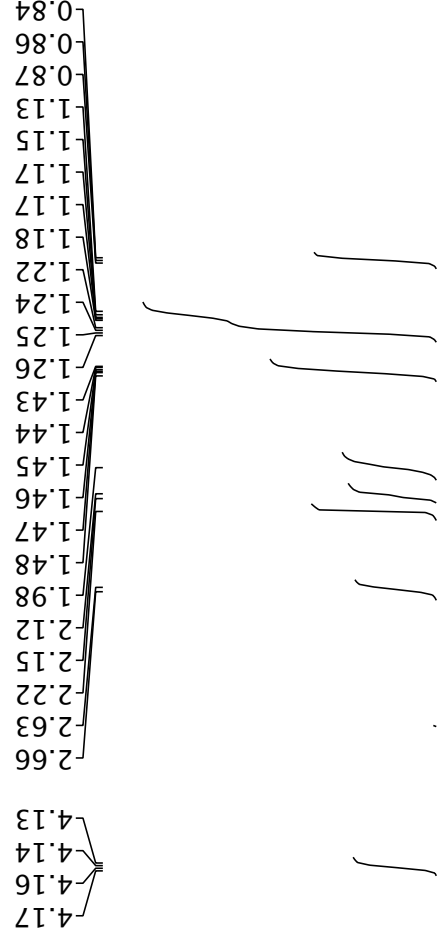
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	19.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	54
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	499.43
Spectral Width	8000.0
Lowest Frequency	-1518.7
Nucleus	¹ H
Acquired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

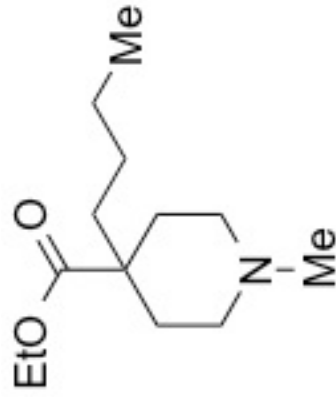




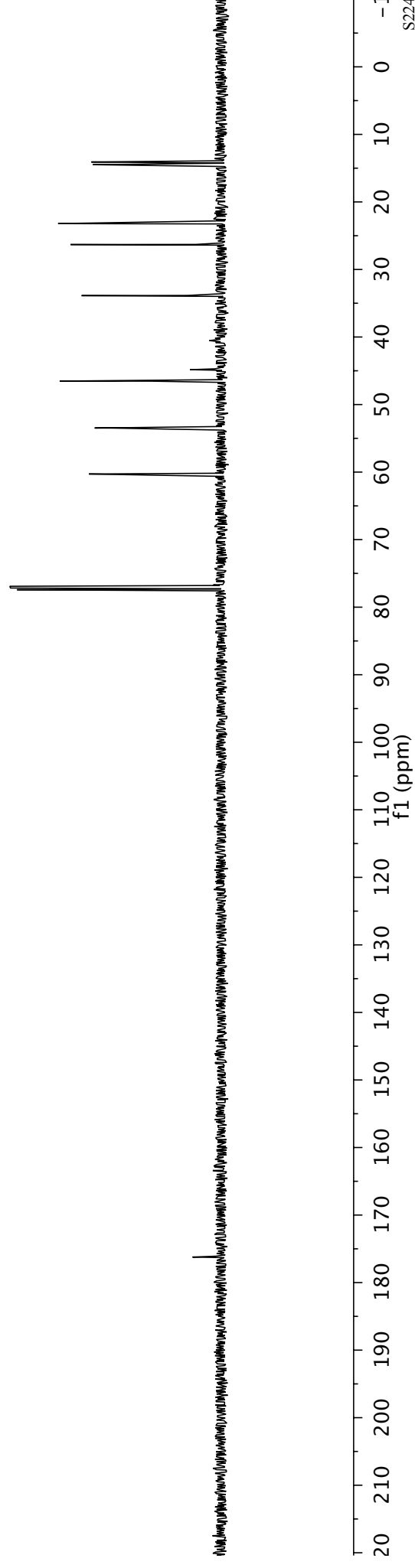
— 7.26 CDCl₃

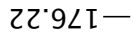
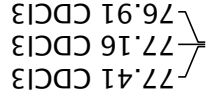
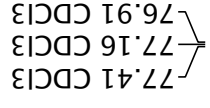
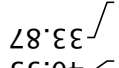
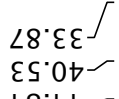
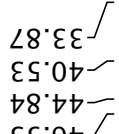
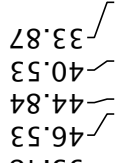
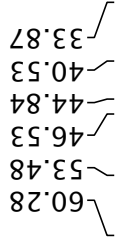
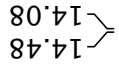
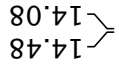
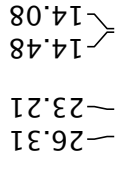
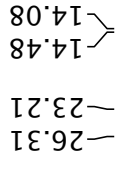
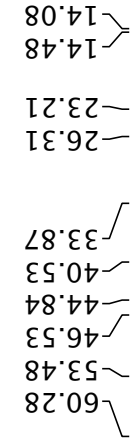
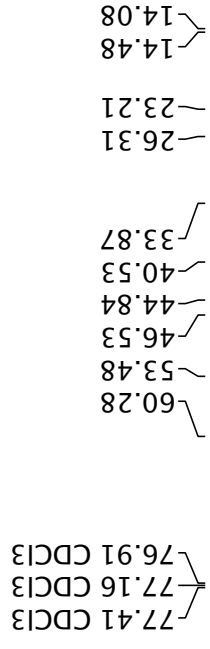
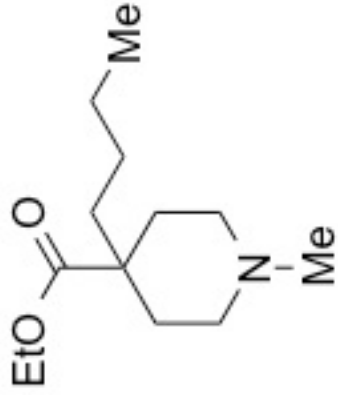
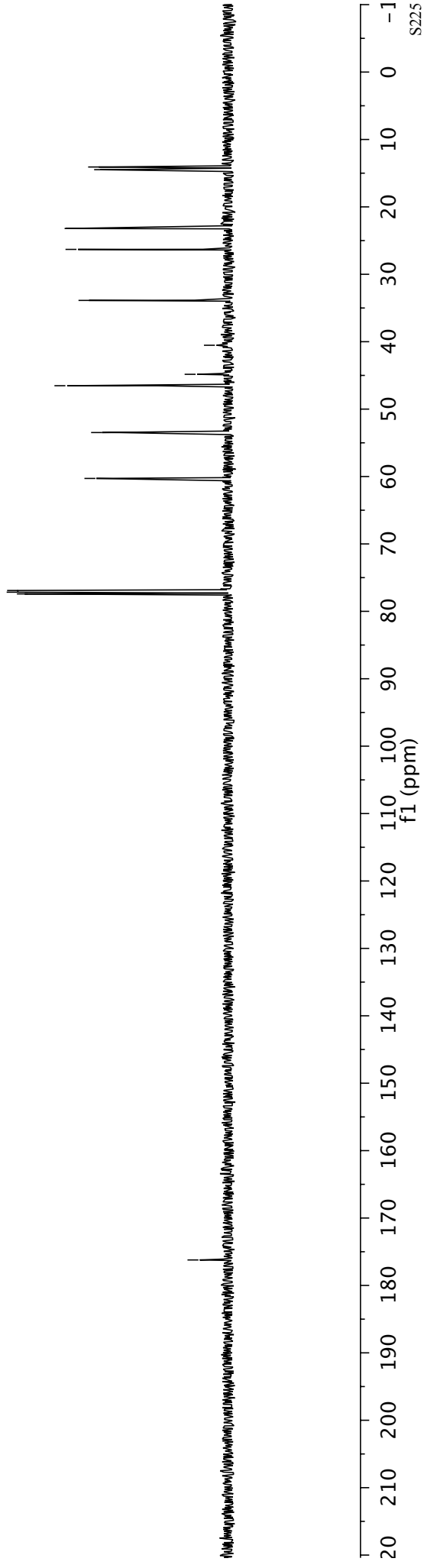
— 5.29 CH₂Cl₂

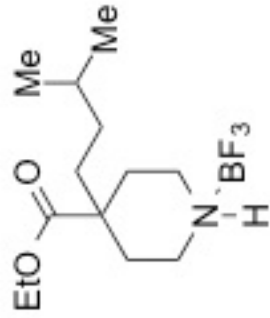




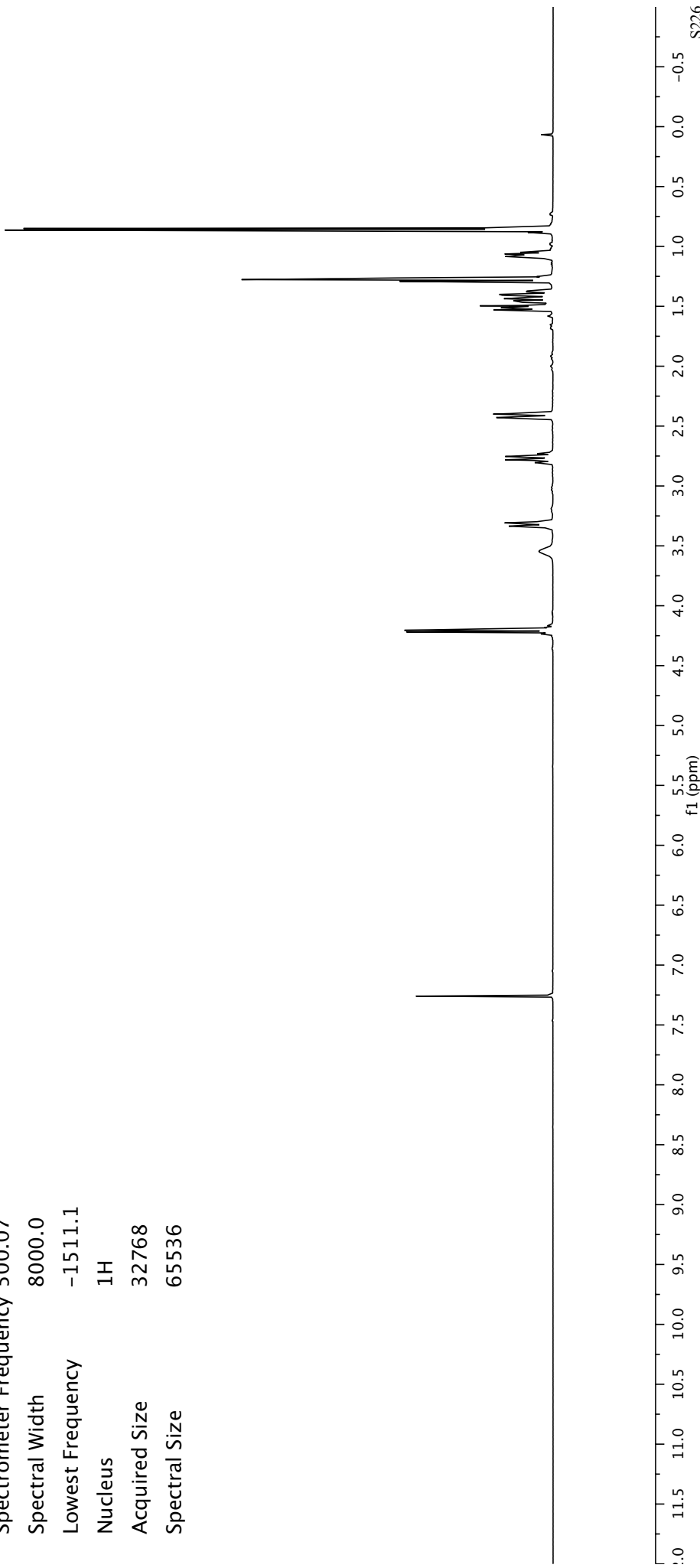
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1272.5
Nucleus	¹³ C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

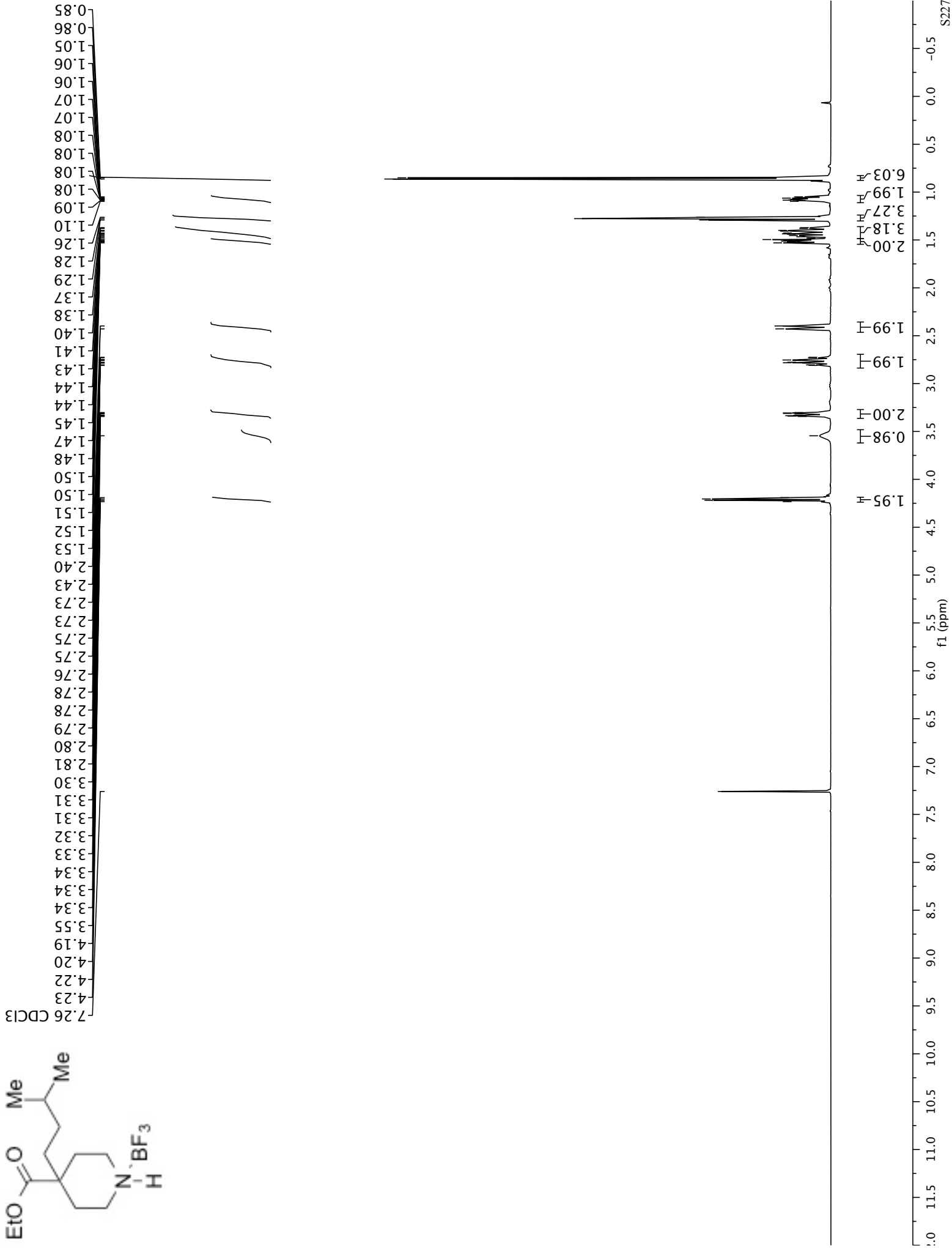
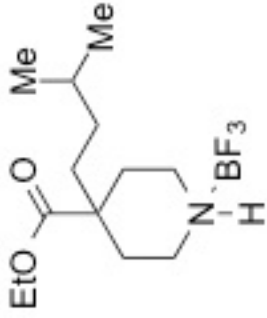


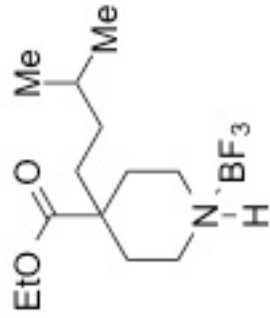




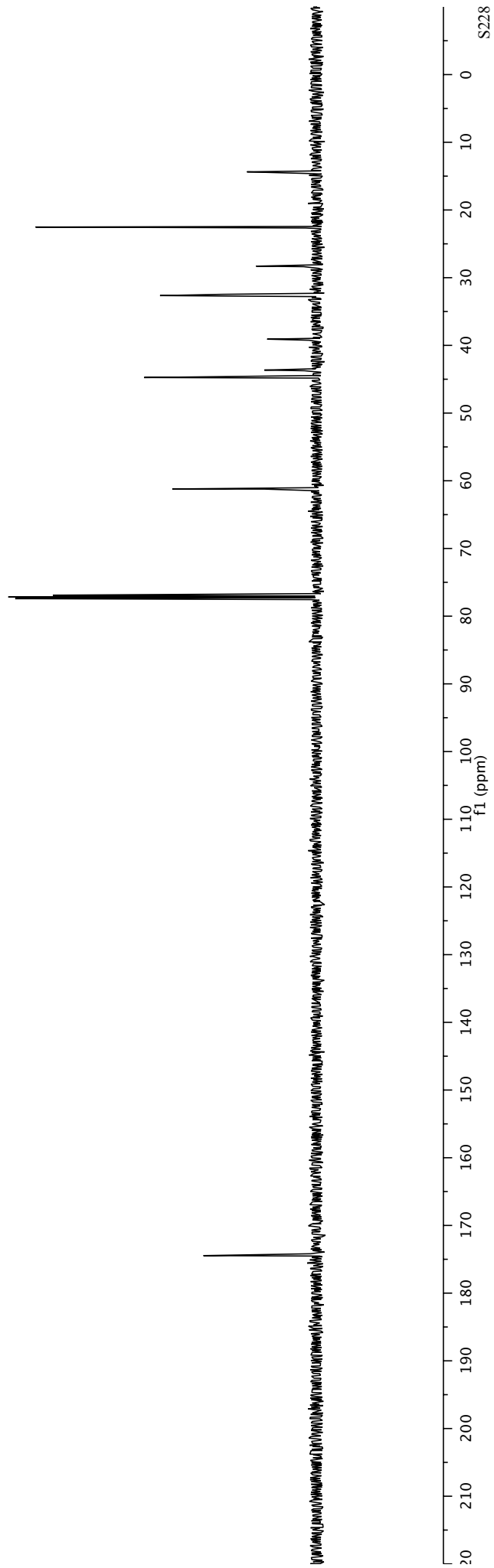
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	32
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1511.1
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

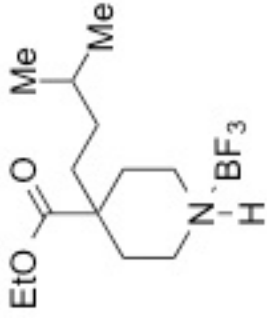






Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Number of Scans	520
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2200.0
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



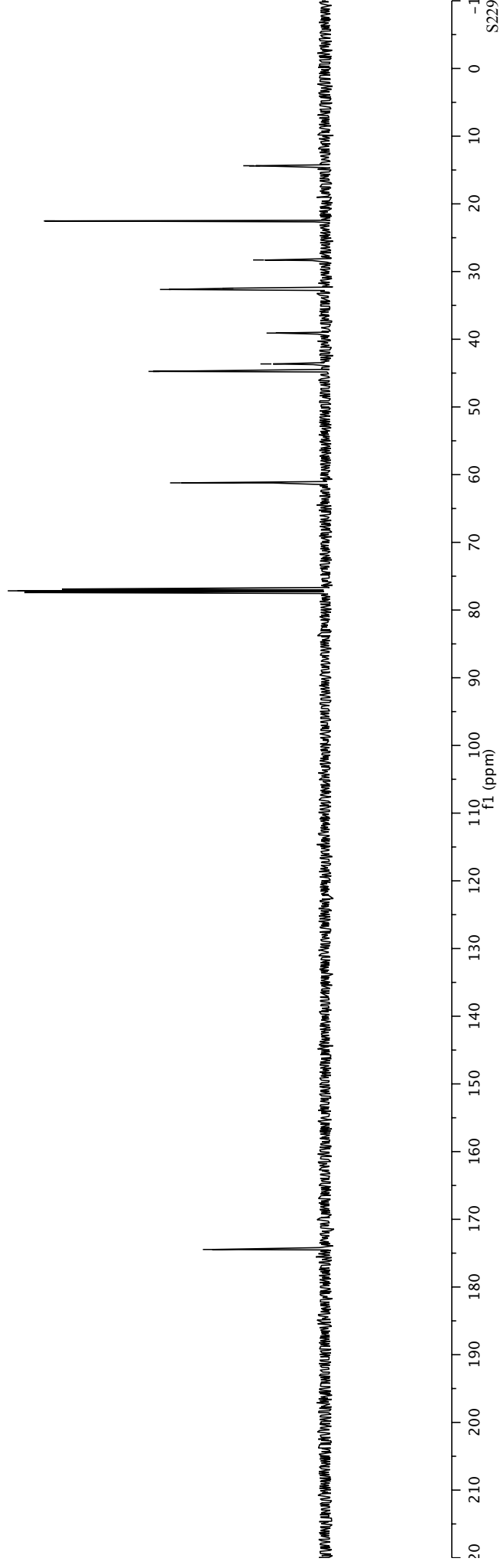


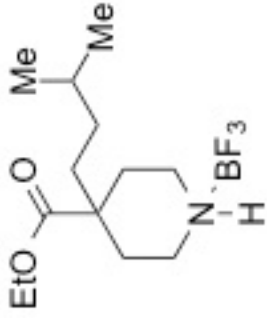
— 174.46

— 77.16 CDCl₃

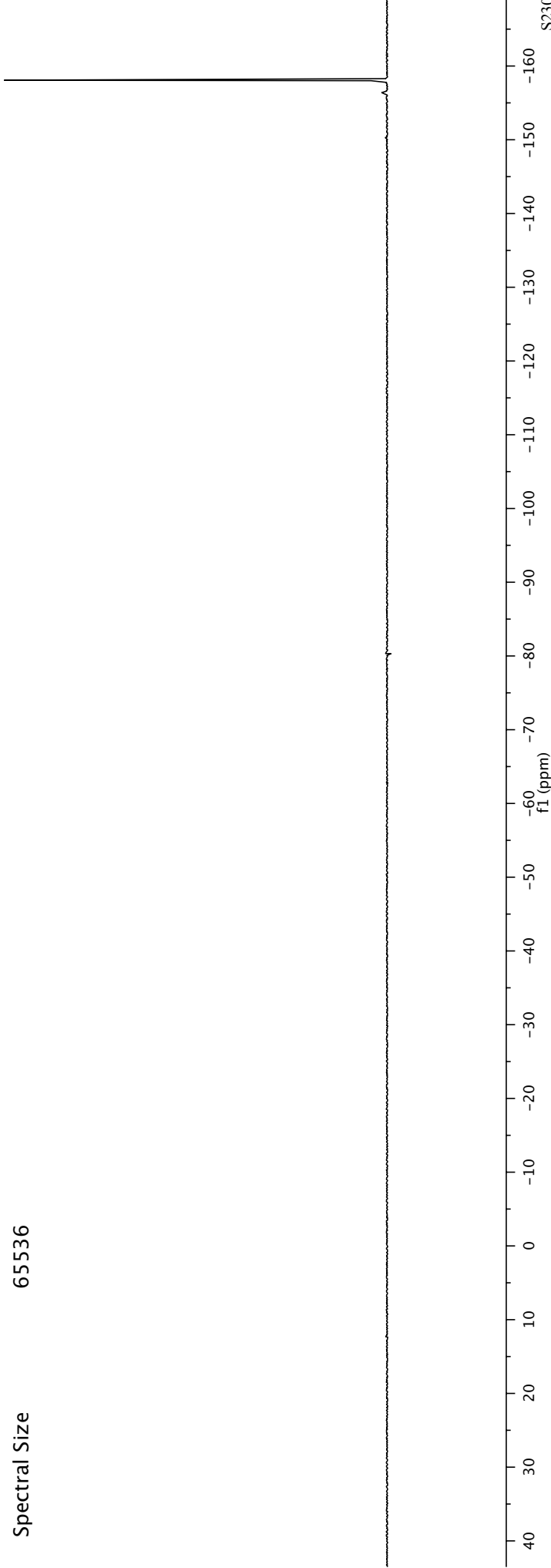
— 61.21

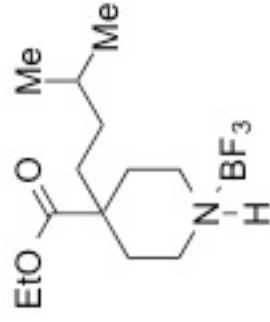
44.75
43.65
39.09
32.65
32.47
28.29
22.53
14.41
14.37



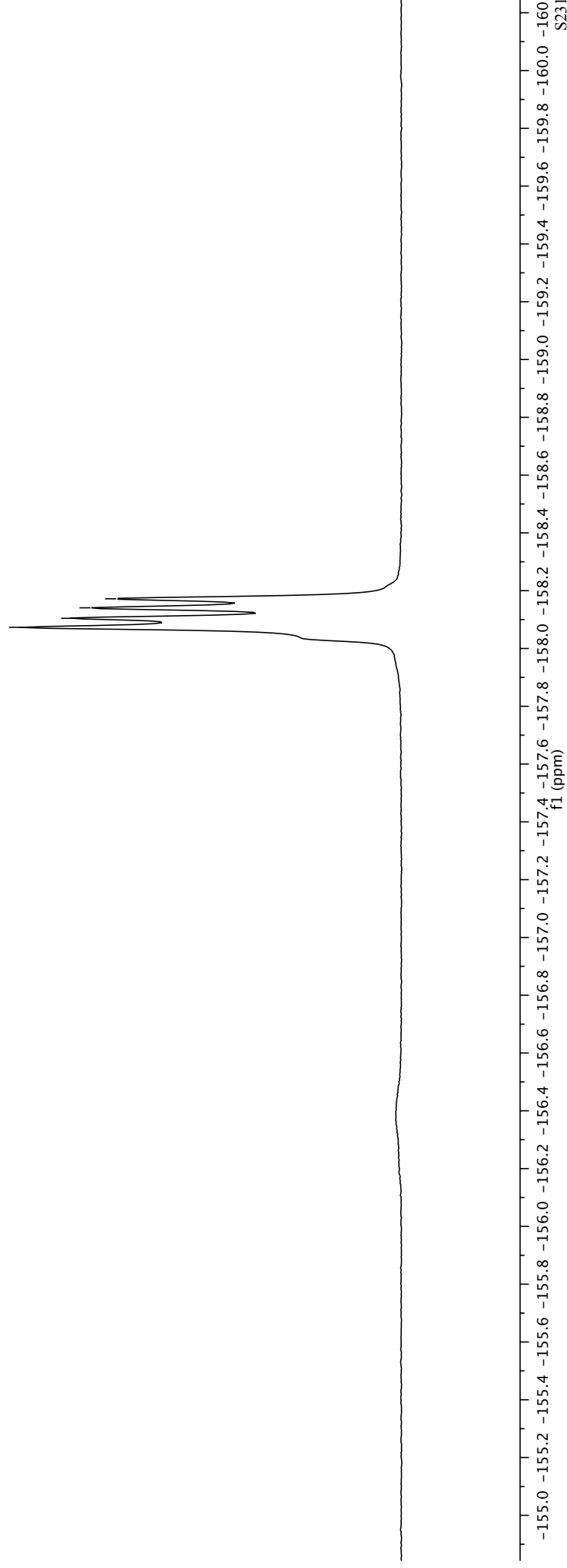


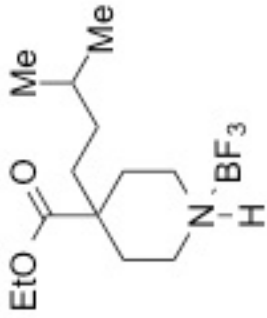
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	120
Receiver Gain	48
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency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



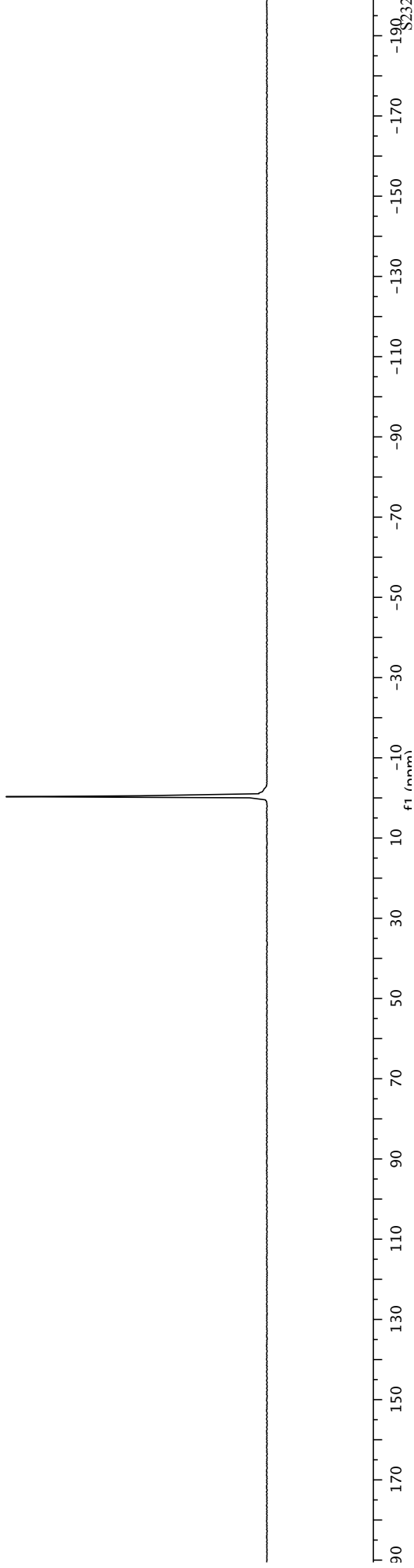


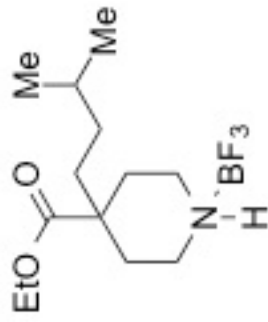
158.07
158.10
158.14
158.17



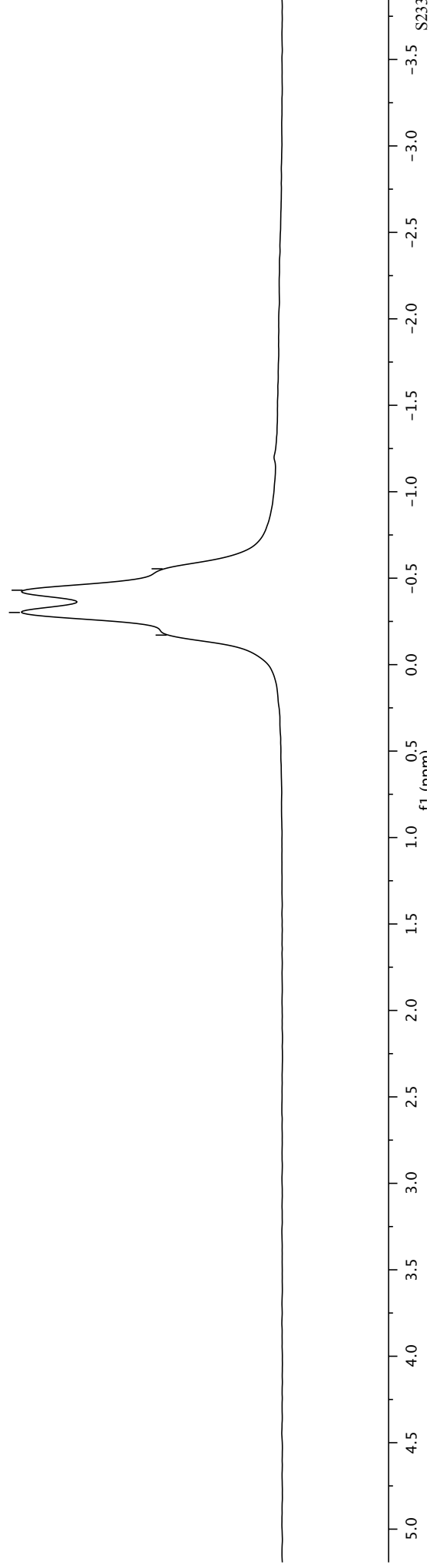


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quadbp
Number of Scans	16
Receiver Gain	58
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.6554
Spectrometer Frequency	128.25
Spectral Width	50000.0
Lowest Frequency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

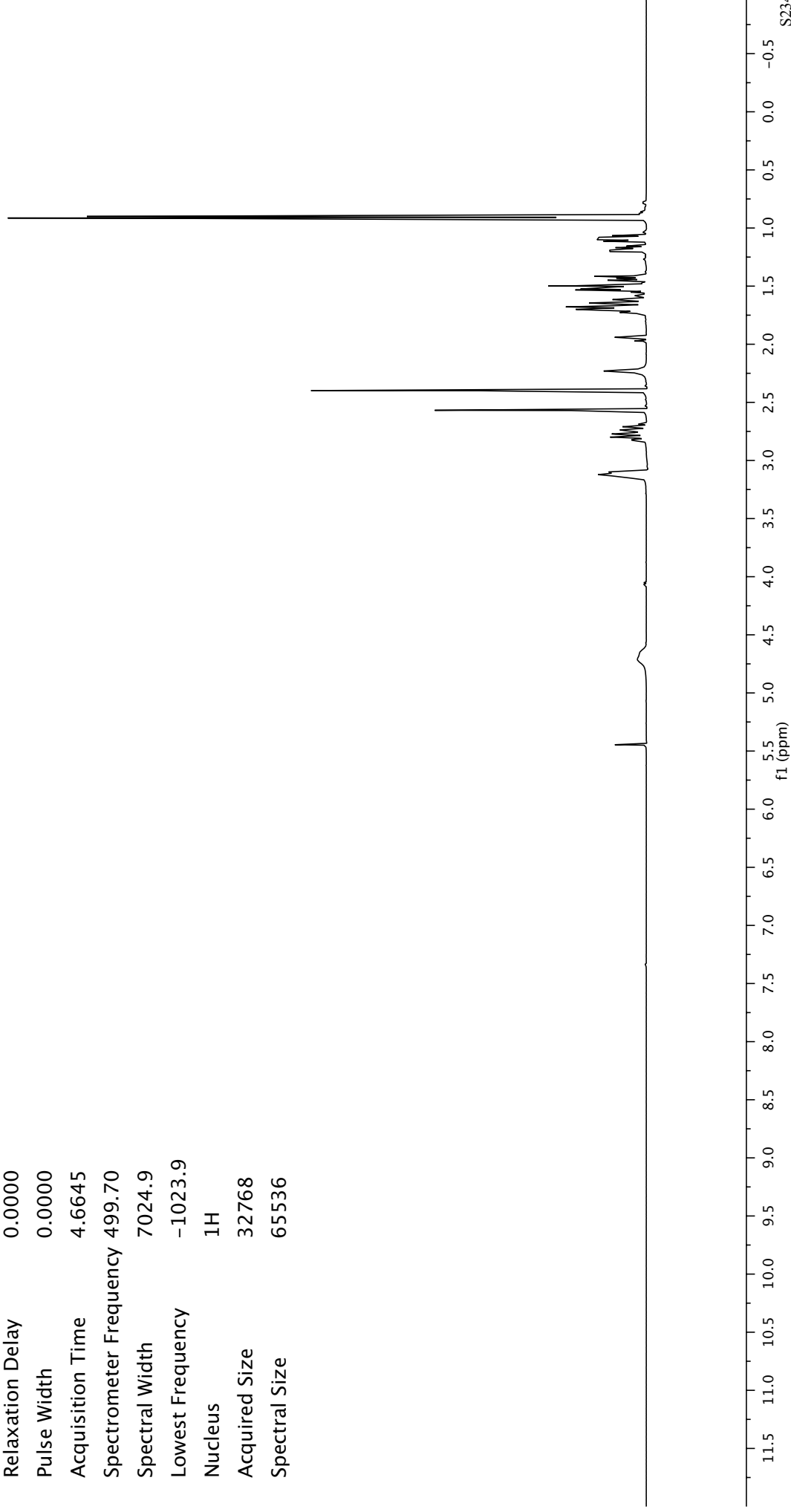
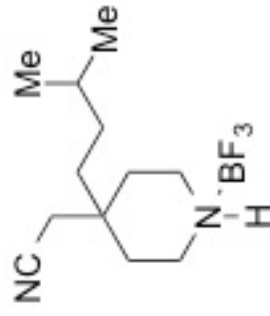




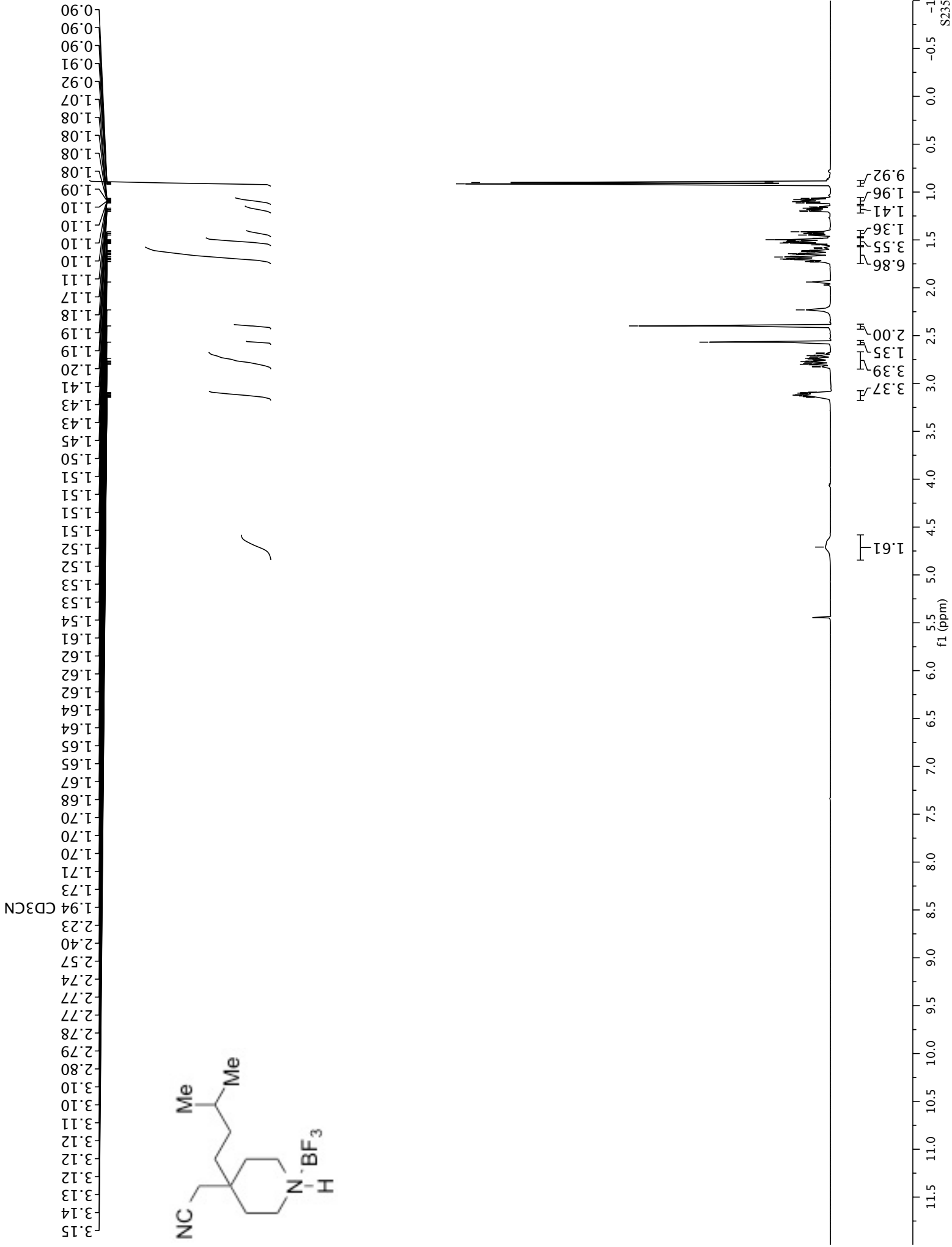
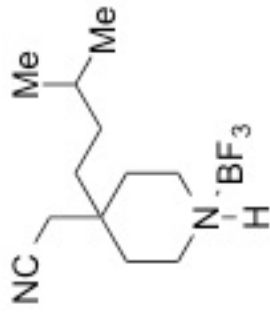
— -0.17
— -0.30
— -0.43
— -0.55

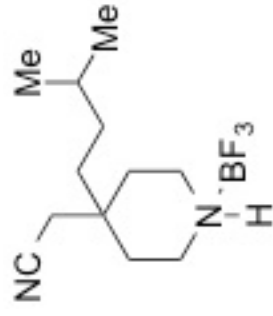


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CD3CN
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	8
Receiver Gain	36
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.70
Spectral Width	7024.9
Lowest Frequency	-1023.9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

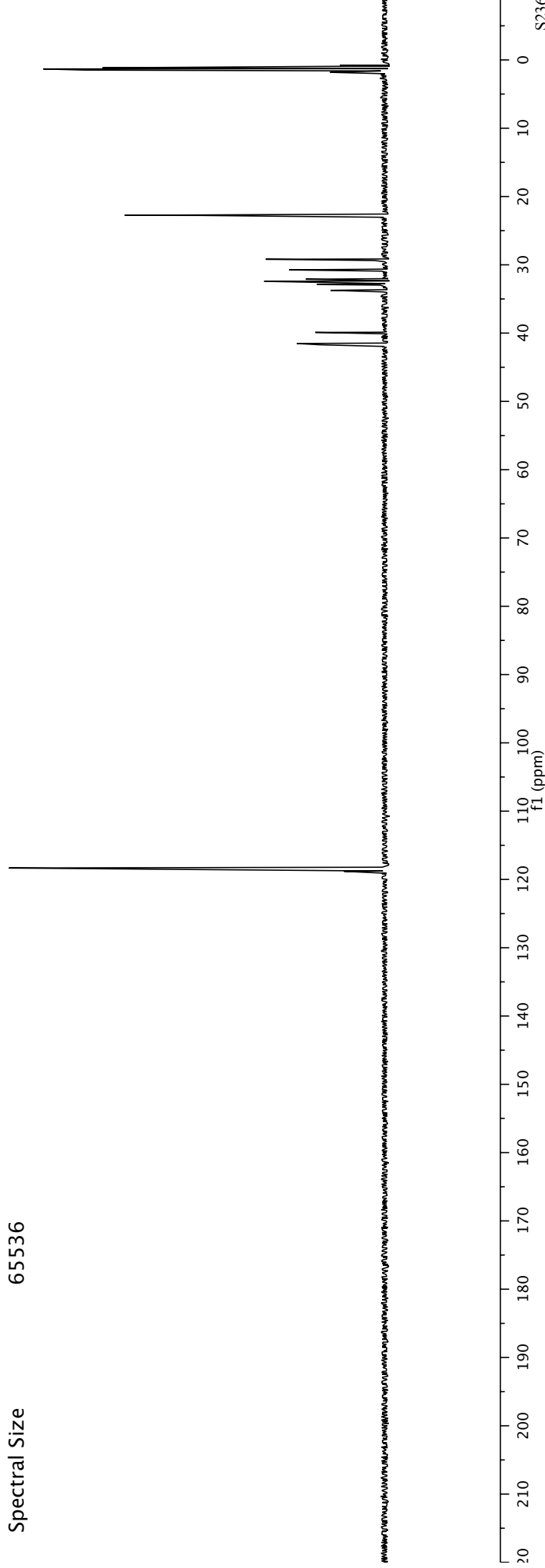


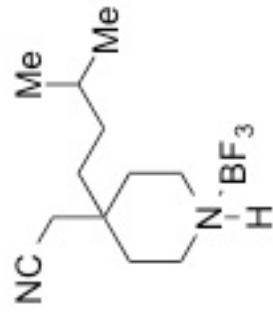
CD3CN





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

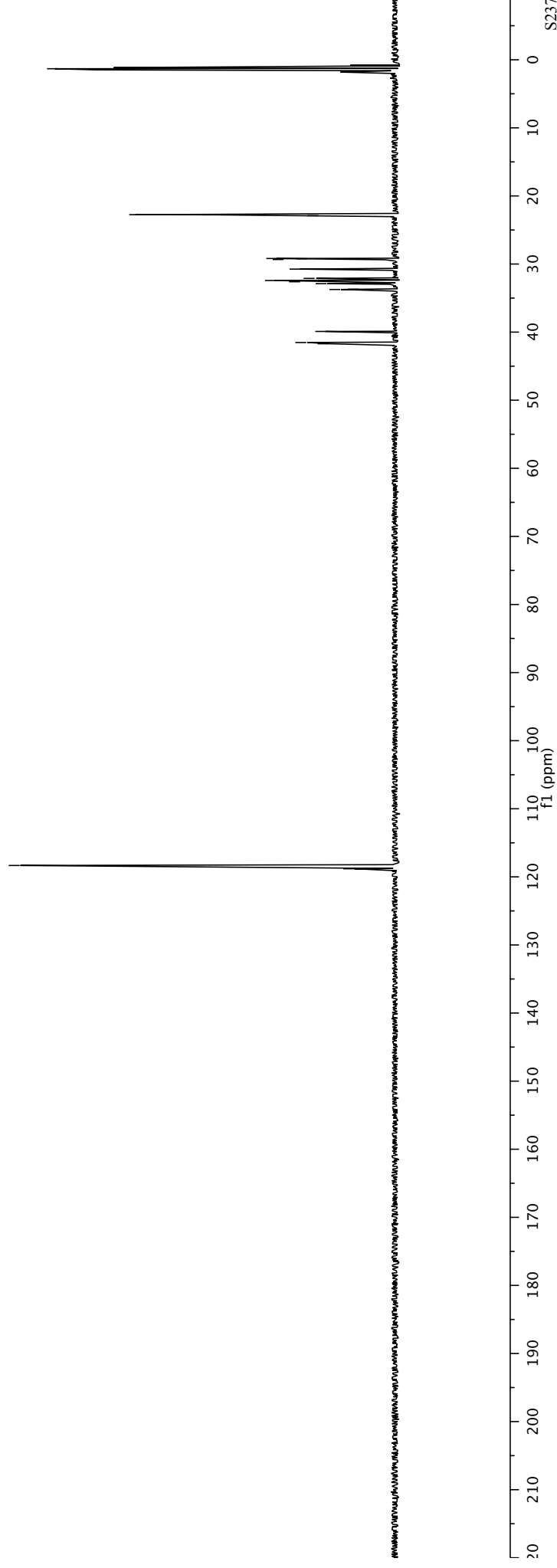


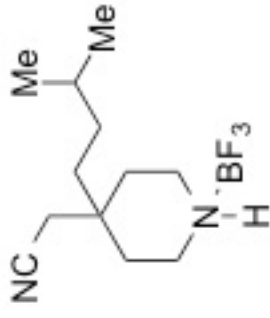


118.87
118.81
118.33

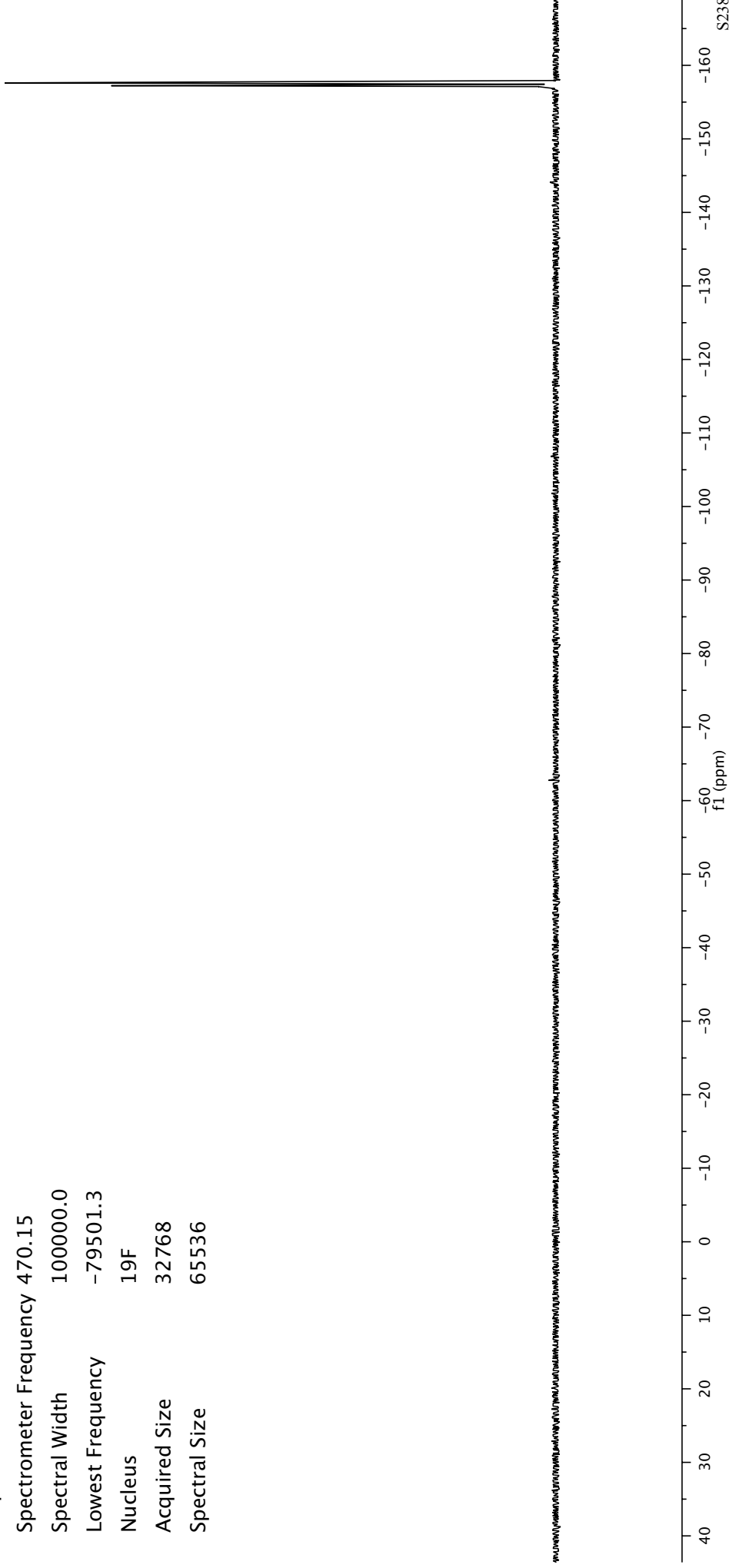
1.32 CD3CN

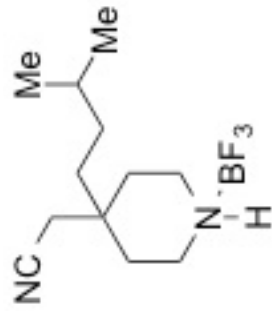
41.71
41.53
39.90
33.74
33.70
32.88
32.60
32.42
32.11
30.75
29.33
29.23
29.19
22.89
22.77
22.75





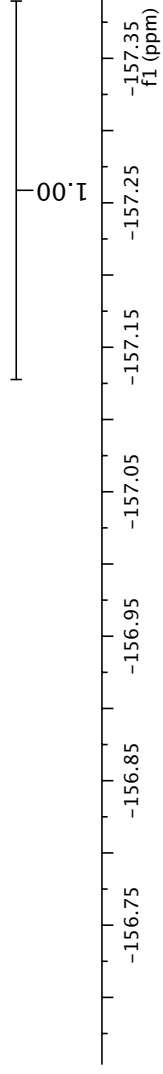
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	64
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency	-79501.3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



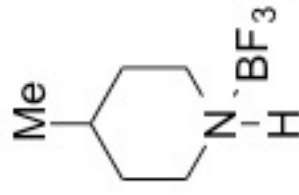


-157.23
 -157.26
 -157.29
 -157.32

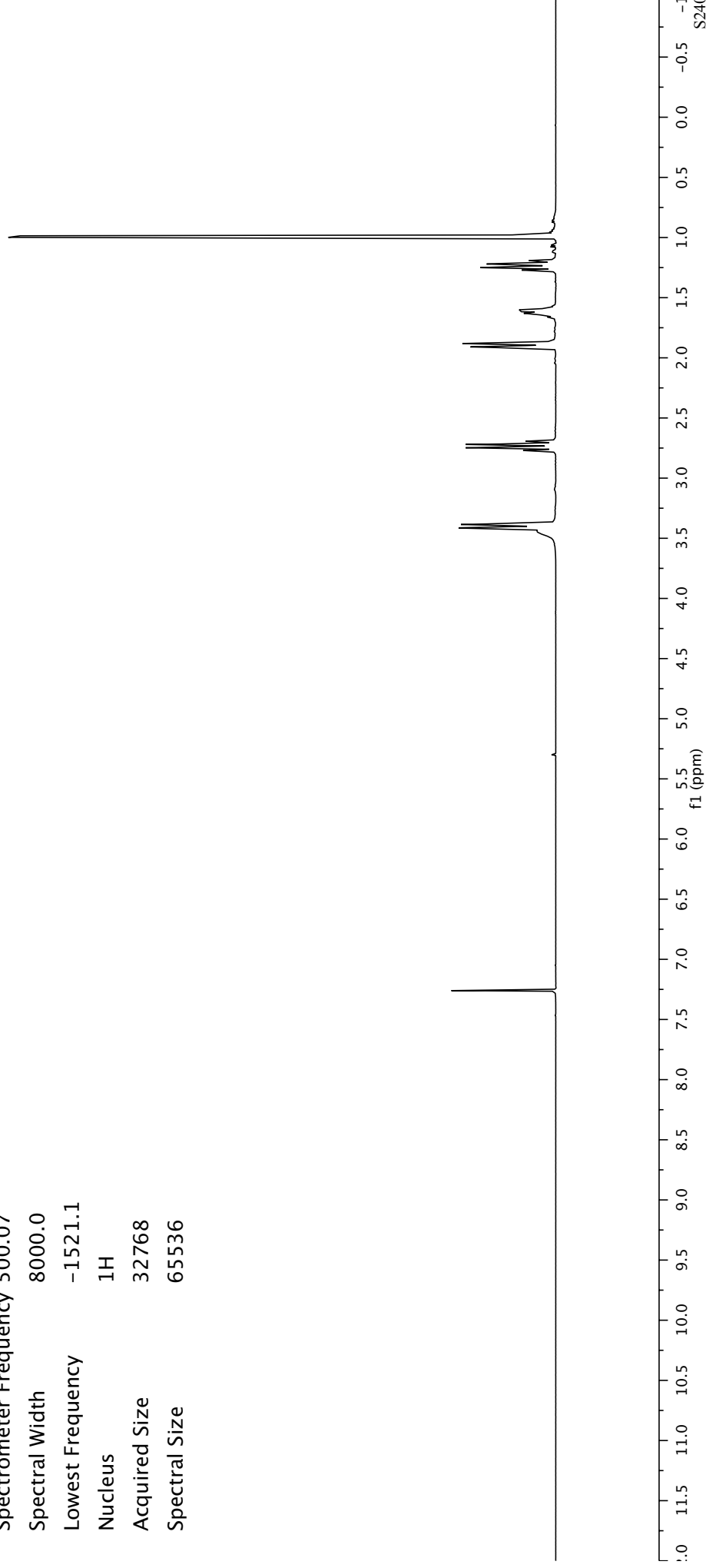
-157.61
 -157.64
 -157.68
 -157.71

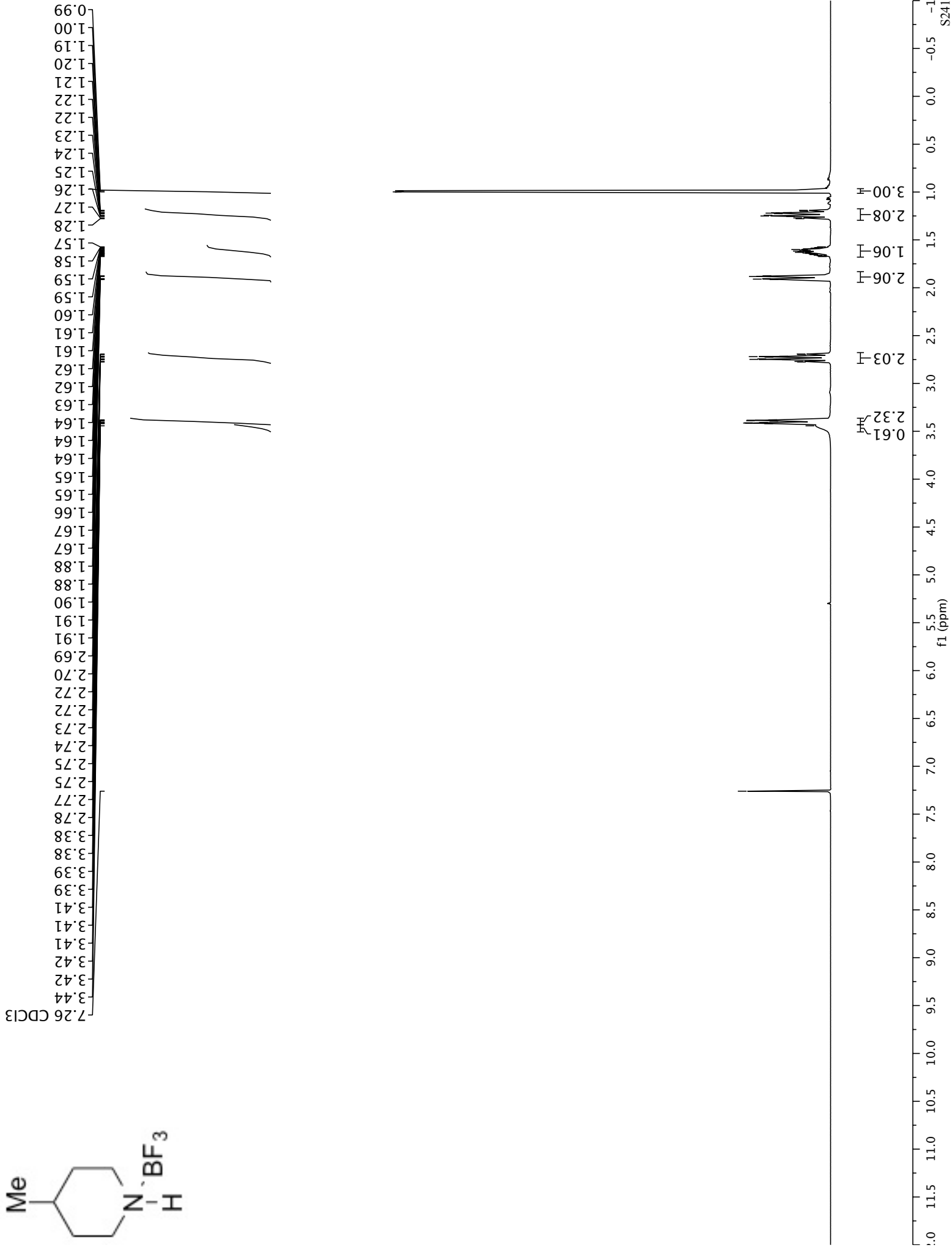
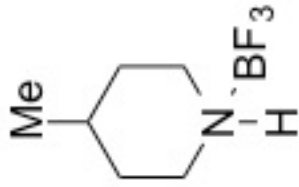


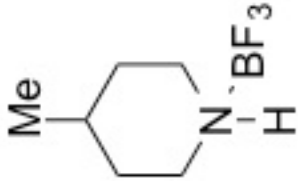
S239



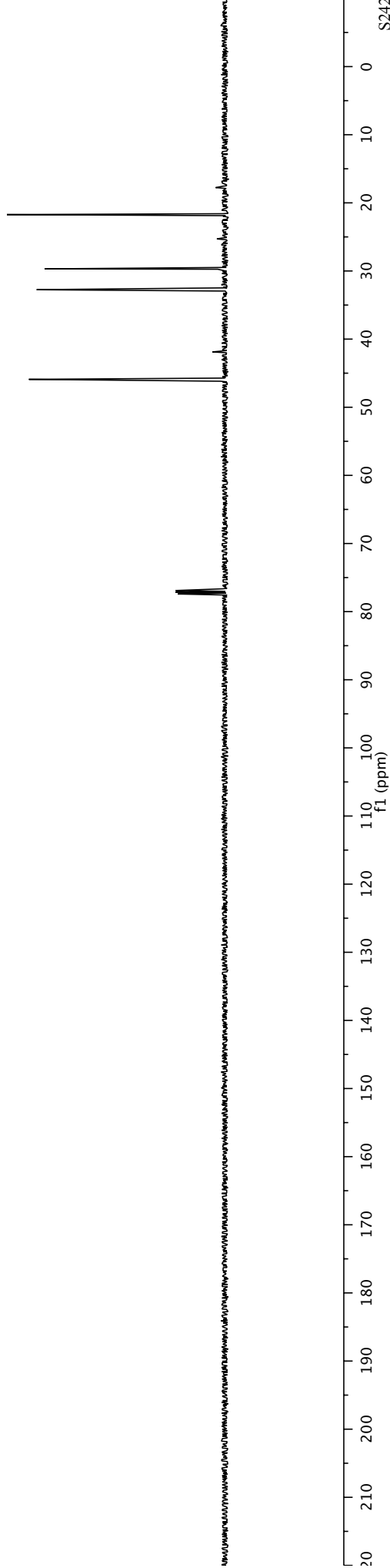
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	32
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1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

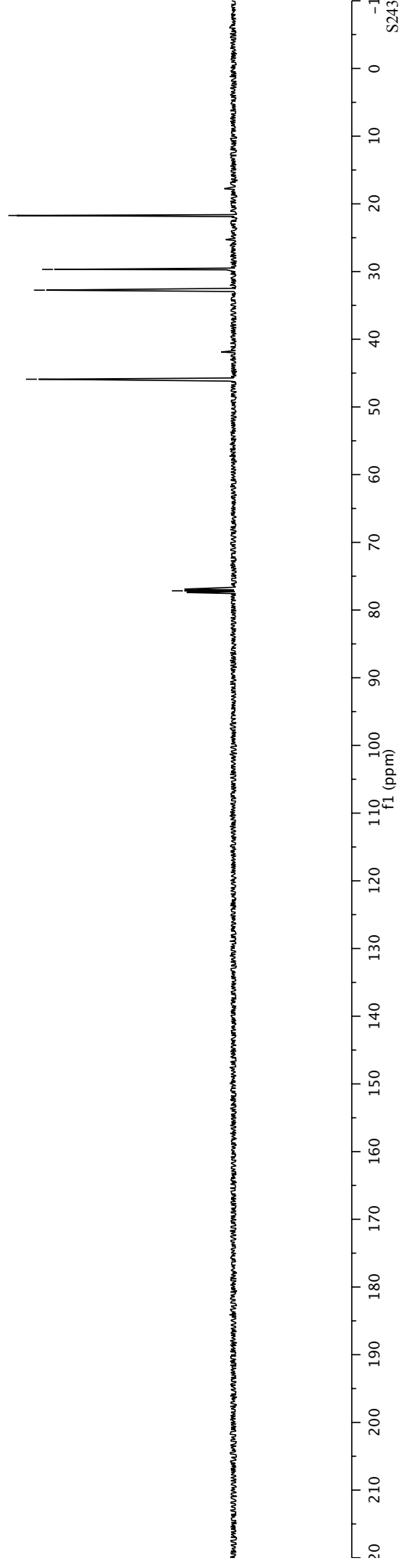
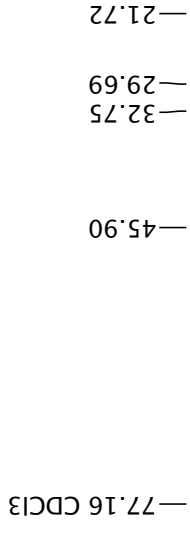
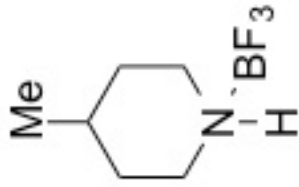


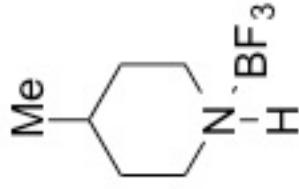




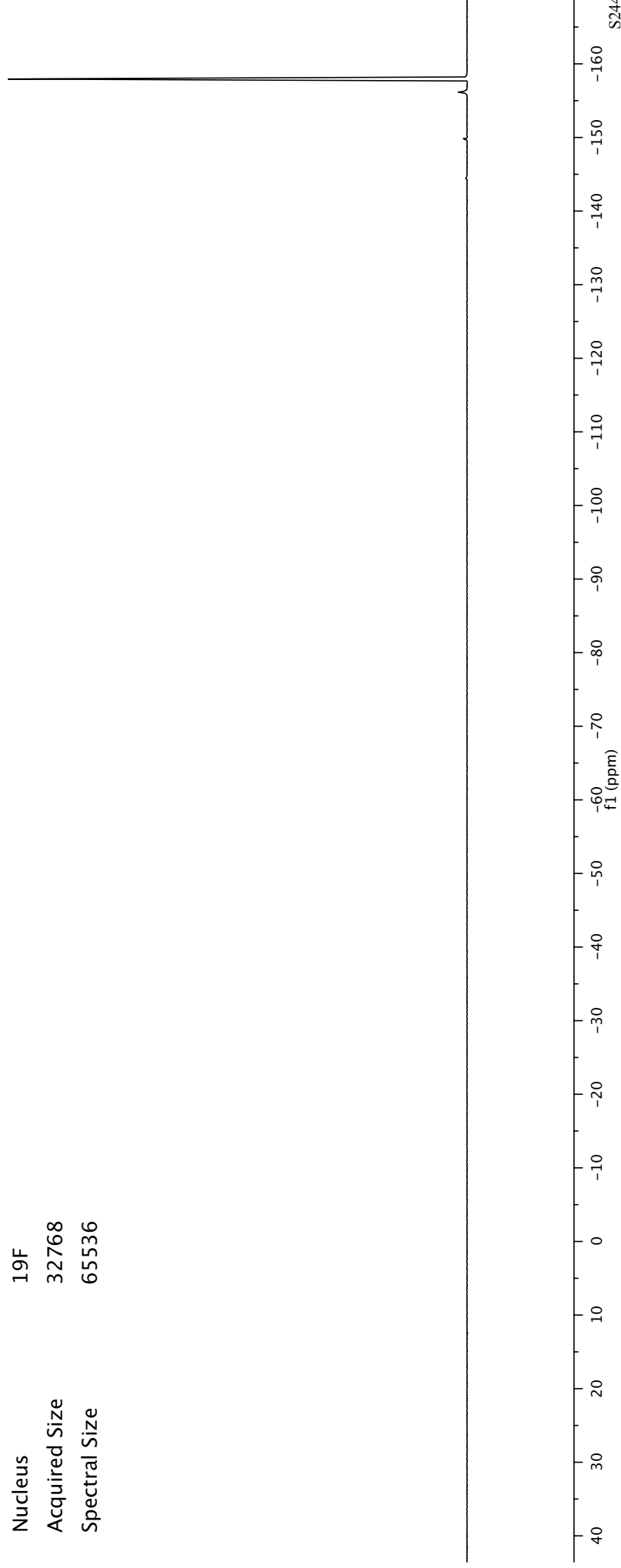
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	64
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1276.5
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

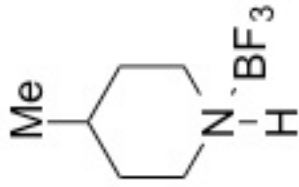




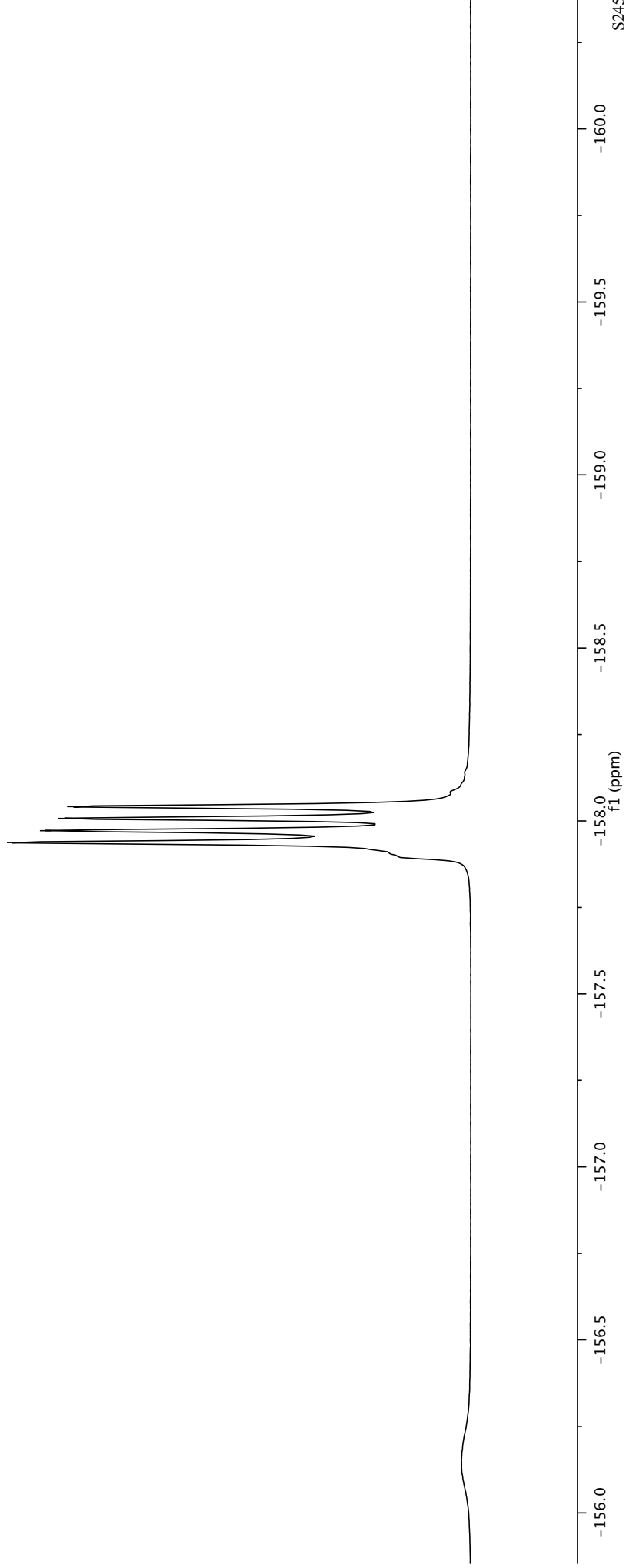


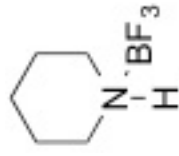
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	64
Receiver Gain	52
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency	-79501.3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



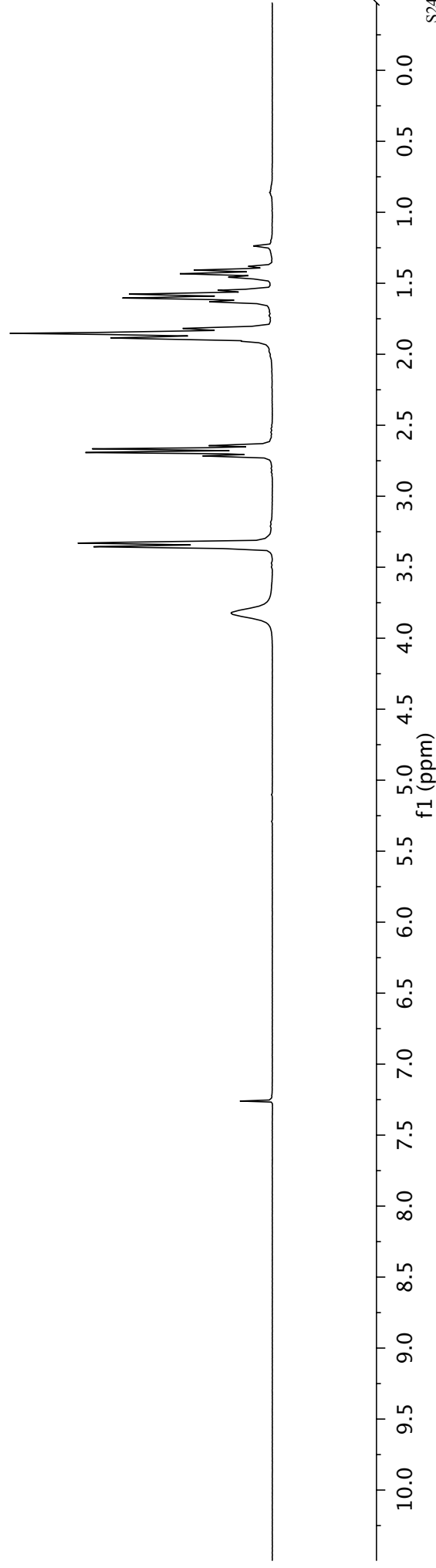


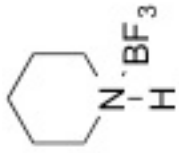
-157.94
-157.97
-158.01
-158.04





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	¹ H
Acquired Size	32768
Spectral Size	65536

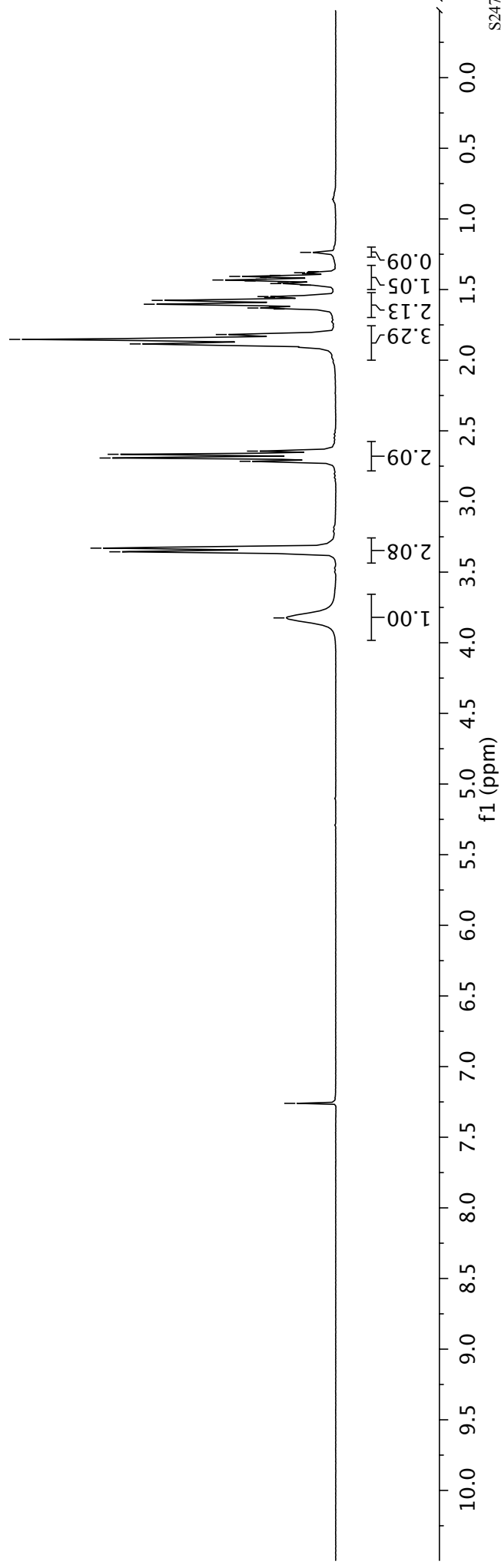
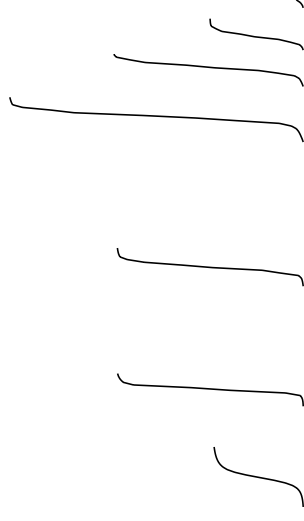


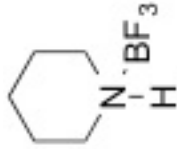


— 7.26 CDCl₃

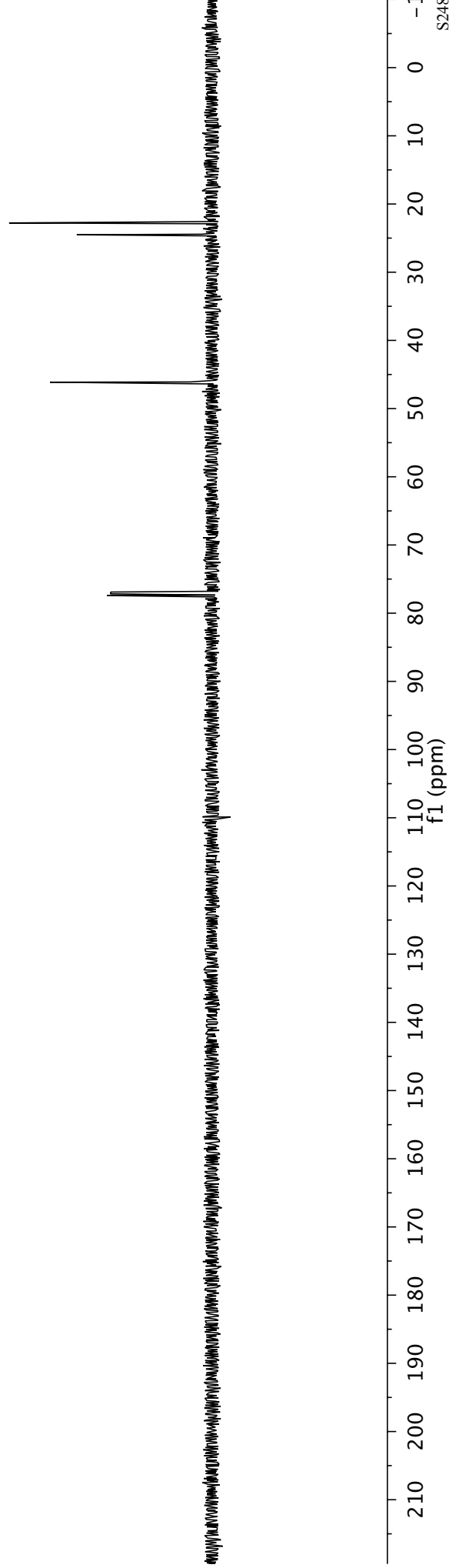
— 3.82
 { 3.36
 { 3.33
 { 2.72
 { 2.69
 { 2.67
 { 2.64

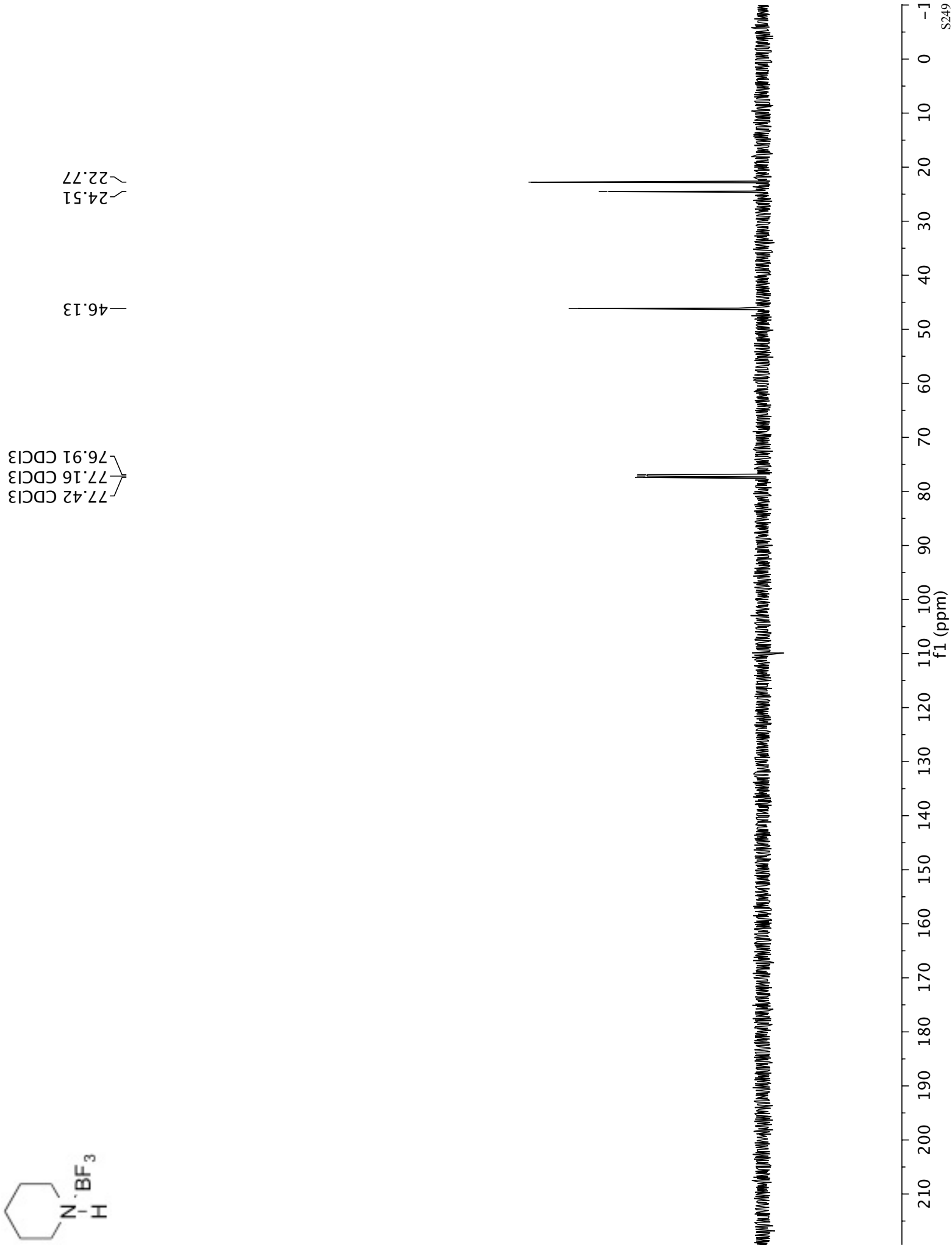
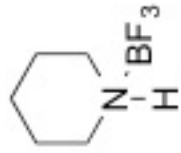
1.88
 { 1.85
 { 1.82
 { 1.63
 { 1.62
 { 1.60
 { 1.58
 { 1.56
 { 1.55
 { 1.44
 { 1.43
 { 1.43
 { 1.41
 { 1.41
 { 1.40

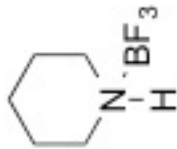




Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1274.6
Nucleus	13C
Acquired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



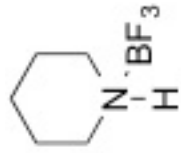




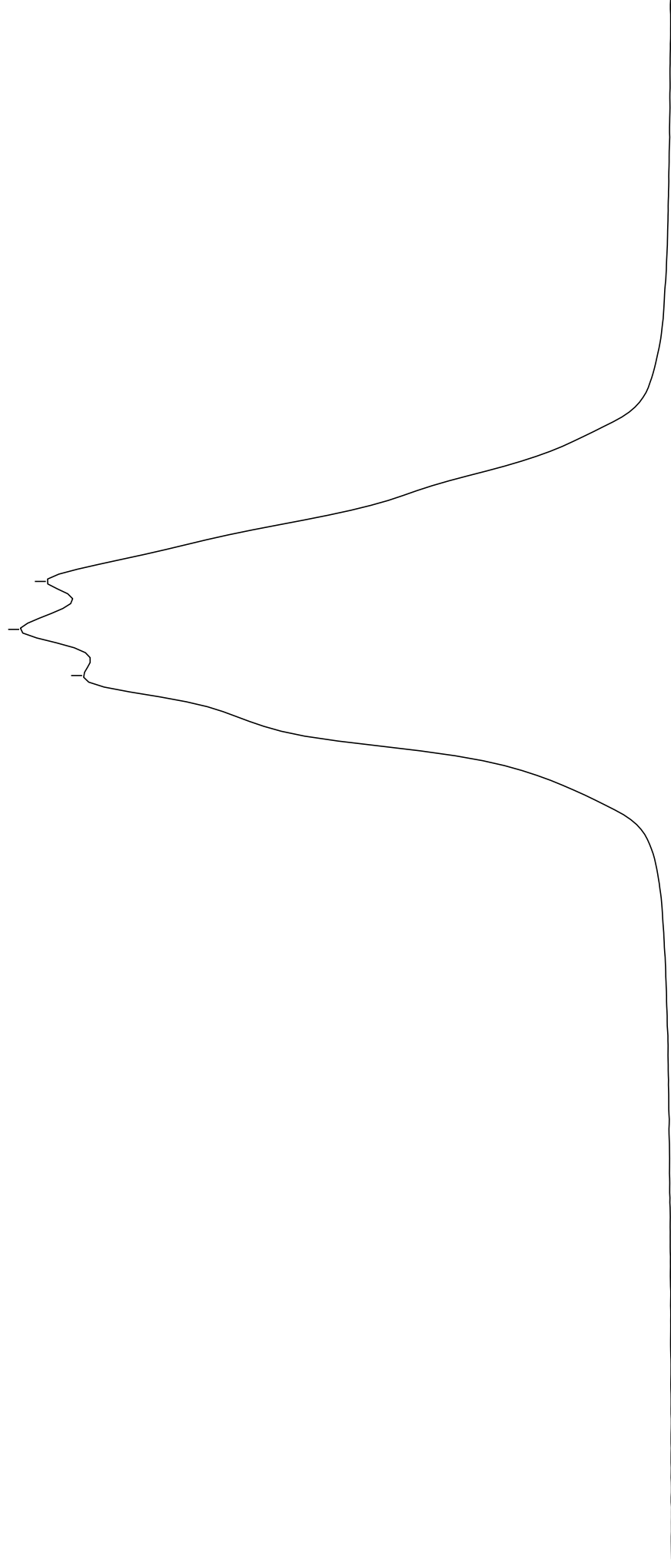
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	50
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency	-79544.1
Nucleus	19F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

f1 (ppm)

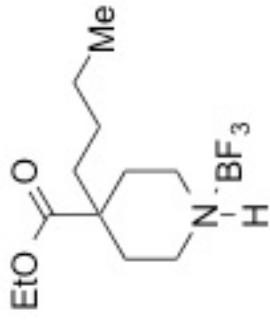
S250



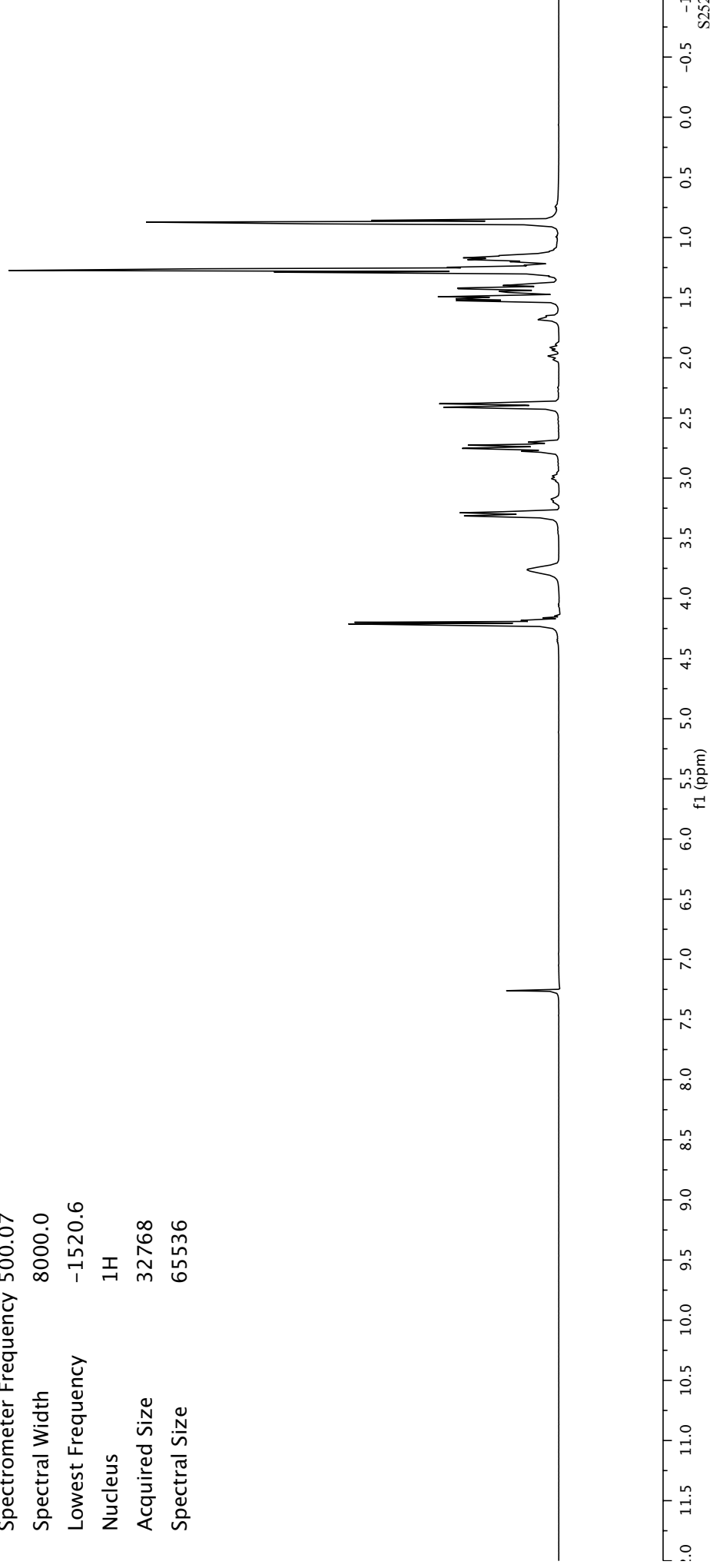
158.20
158.23
158.27

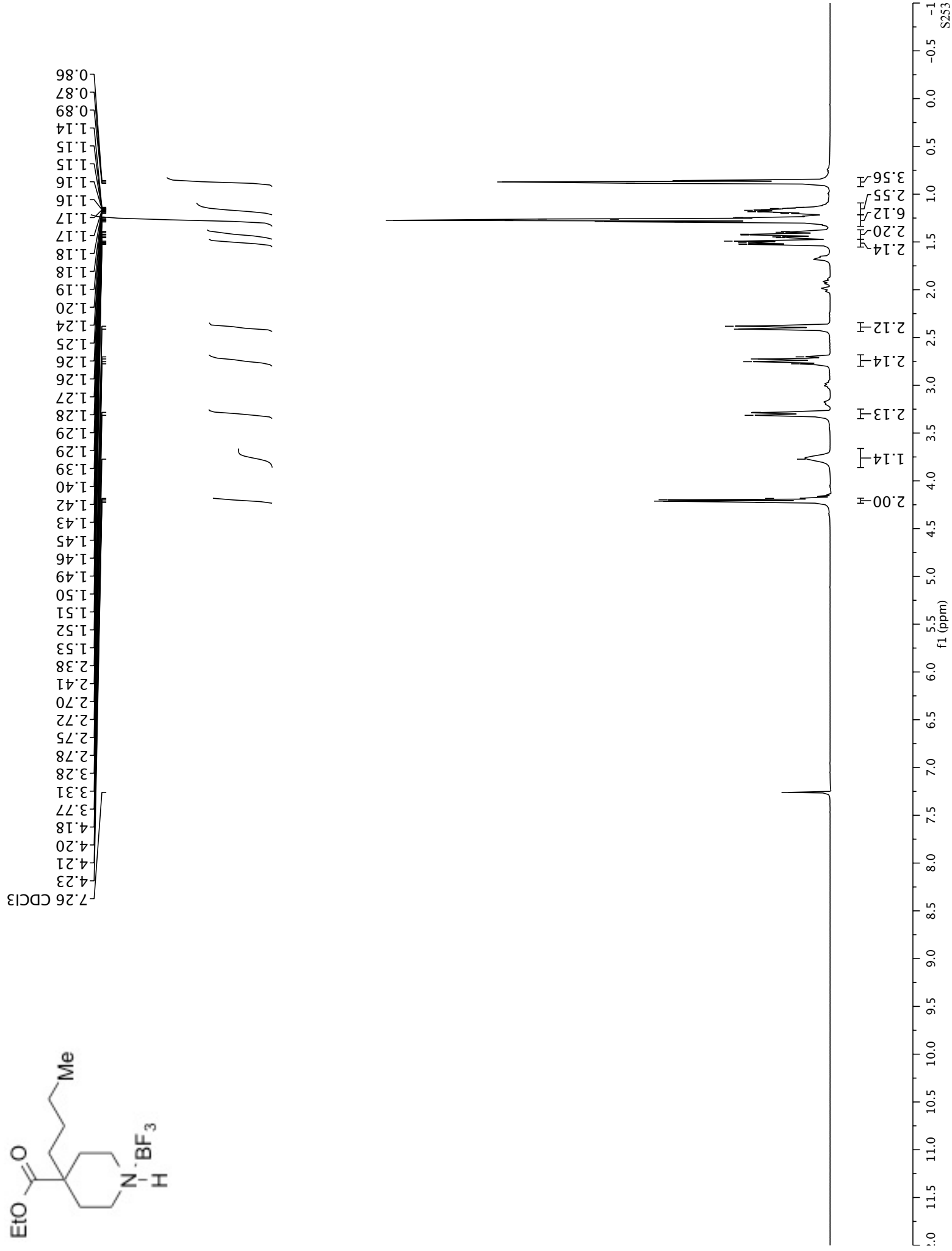
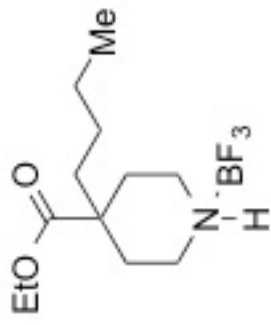


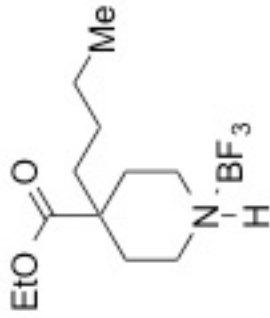
-157.65 -157.75 -157.85 -157.95 -158.05 -158.15 -158.20 -158.23 -158.25 -158.35 -158.45 -158.55 -158.65
f1 (ppm)
S251



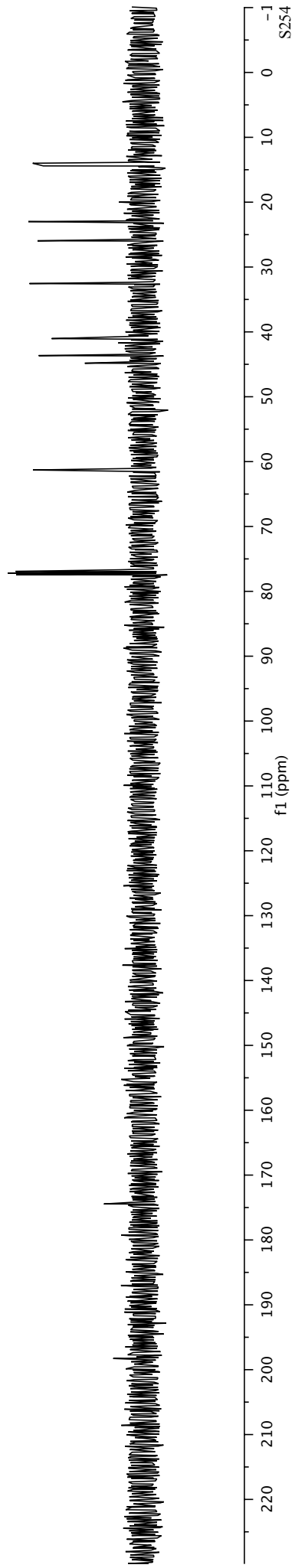
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	26
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1520.6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

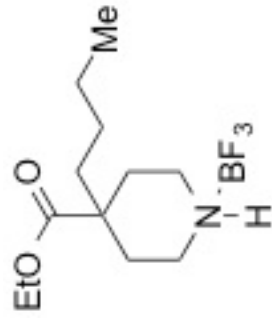






Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	222
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1270.5
Nucleus	13C
Acquired Size	32768
Spectral Size	65536





— 174.45

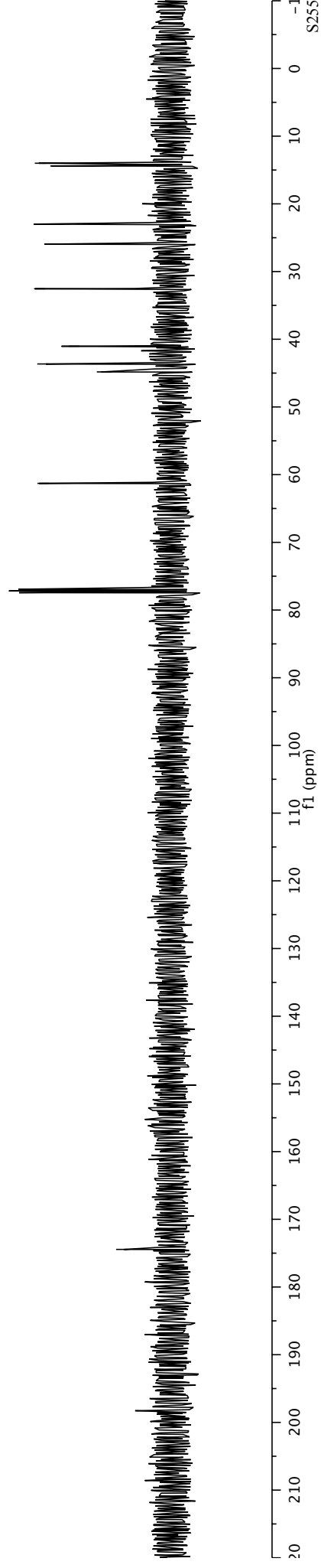
— 77.16 CDCl₃

— 61.29

44.82
43.65
41.03

32.54
25.95
22.99

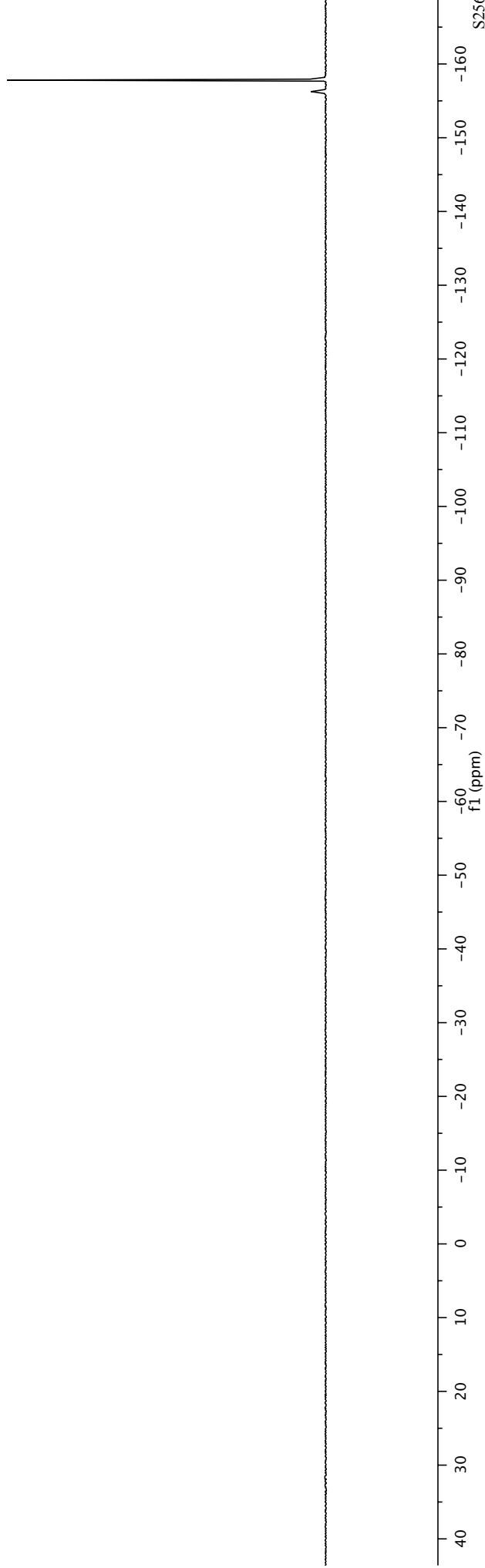
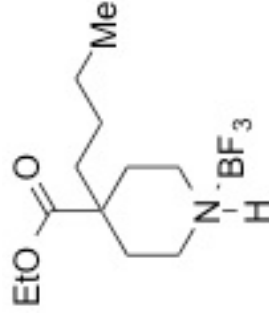
14.40
14.00

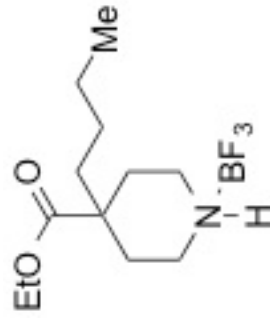


Parameter

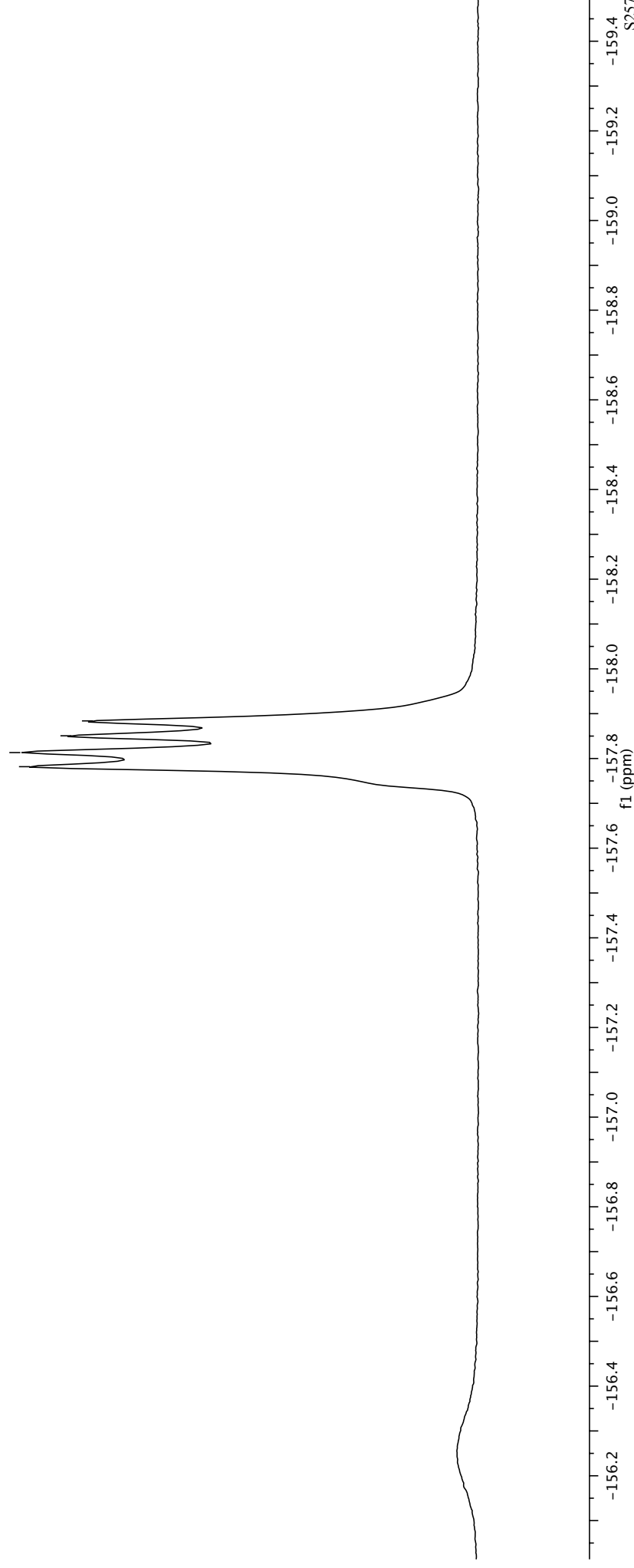
Value

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

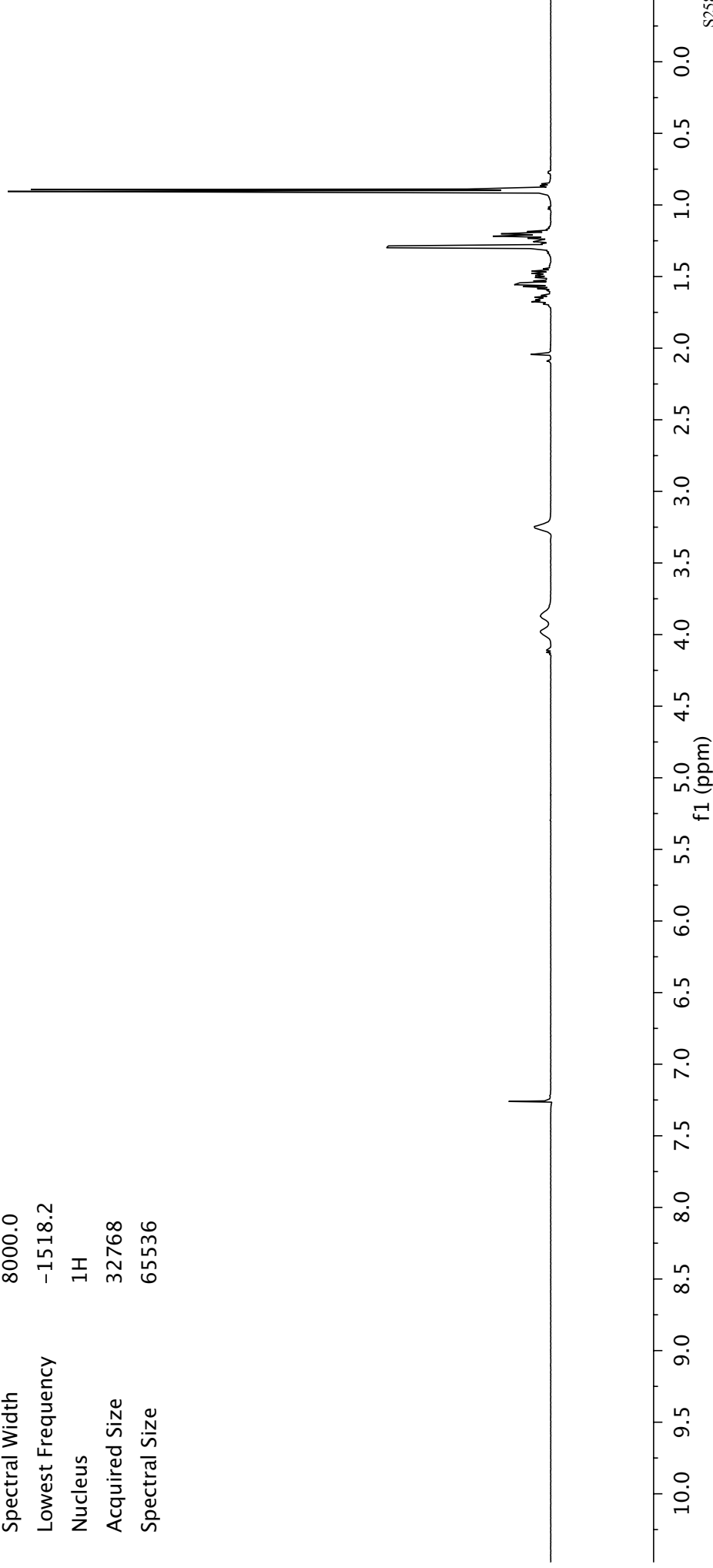
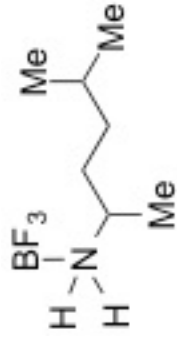


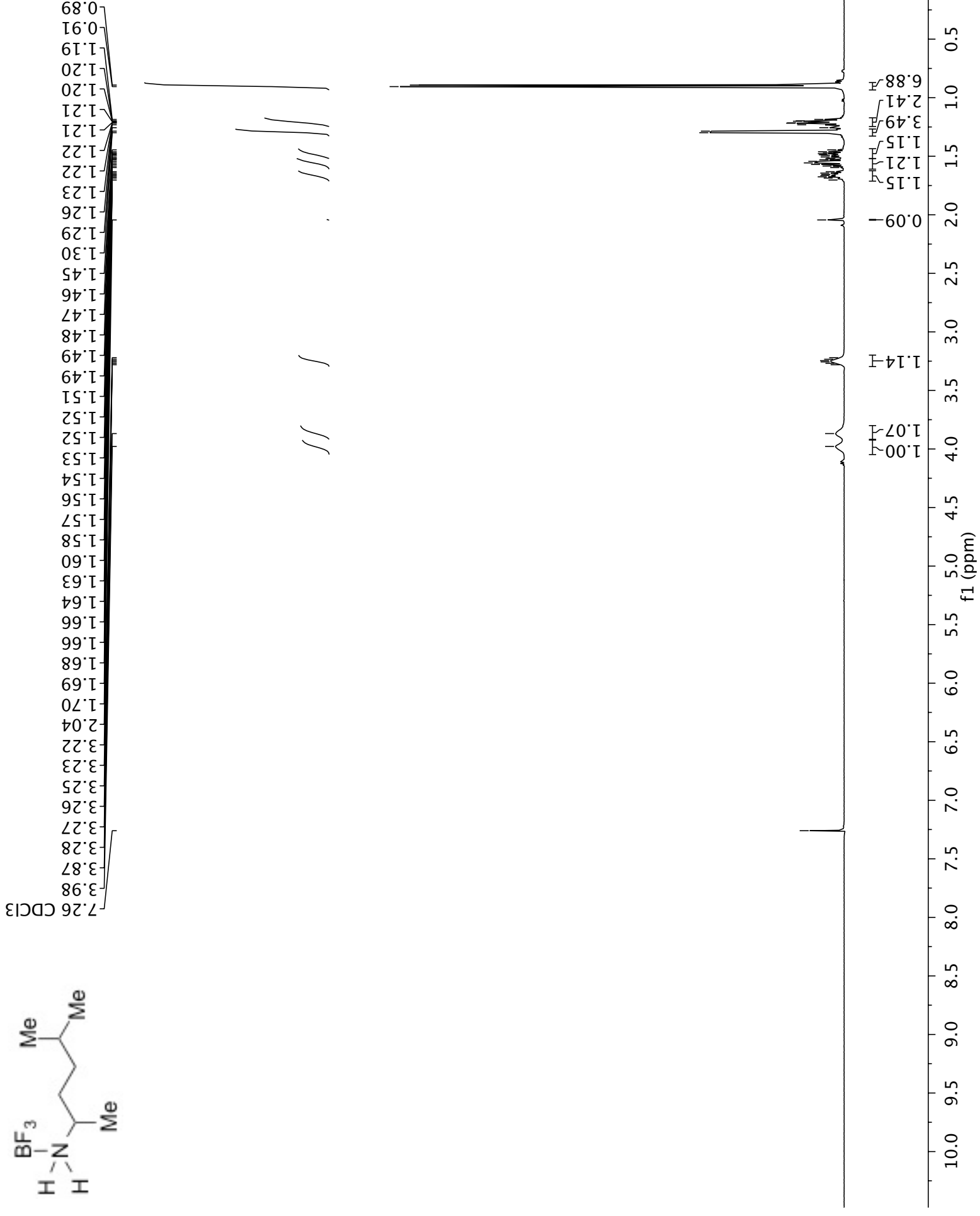
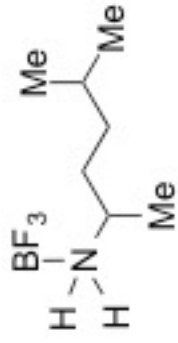


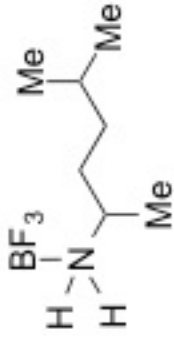
-157.78
-157.81
-157.85
-157.88



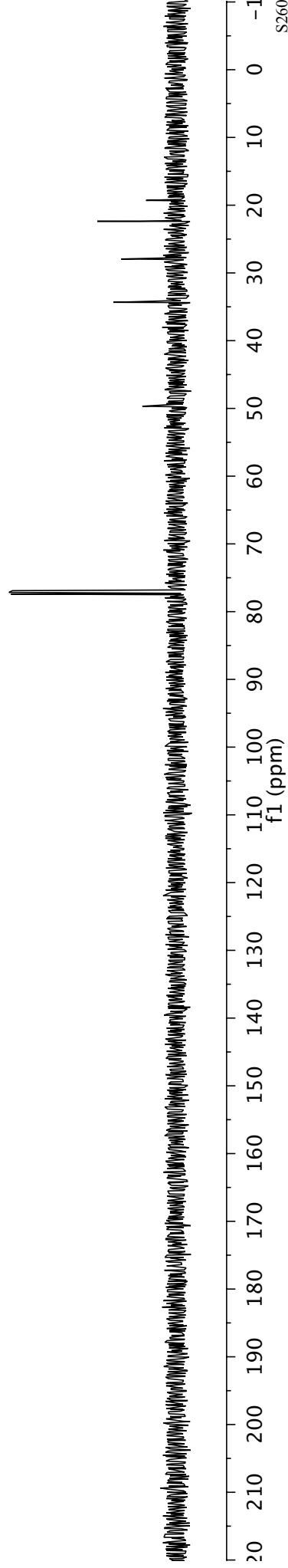
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	52
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	499.43
Spectral Width	8000.0
Lowest Frequency	-1518.2
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

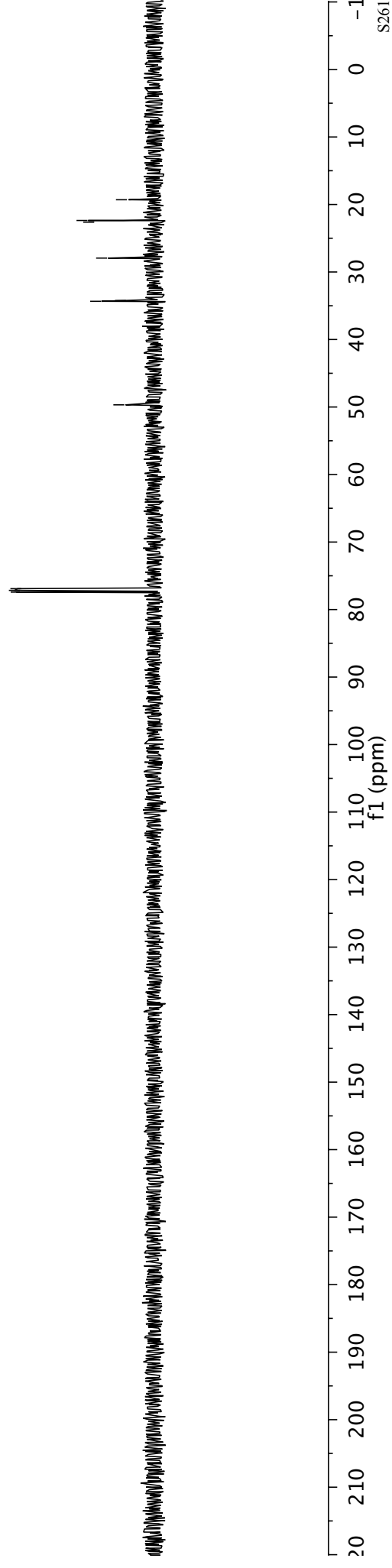
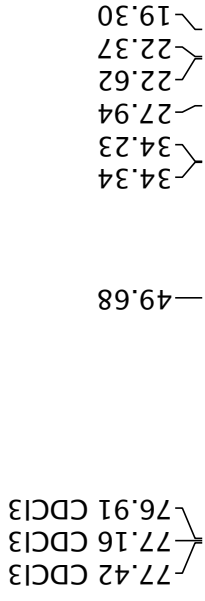
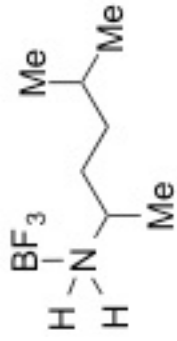


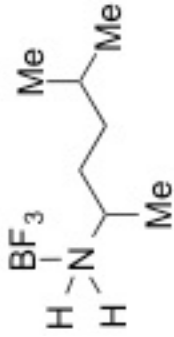




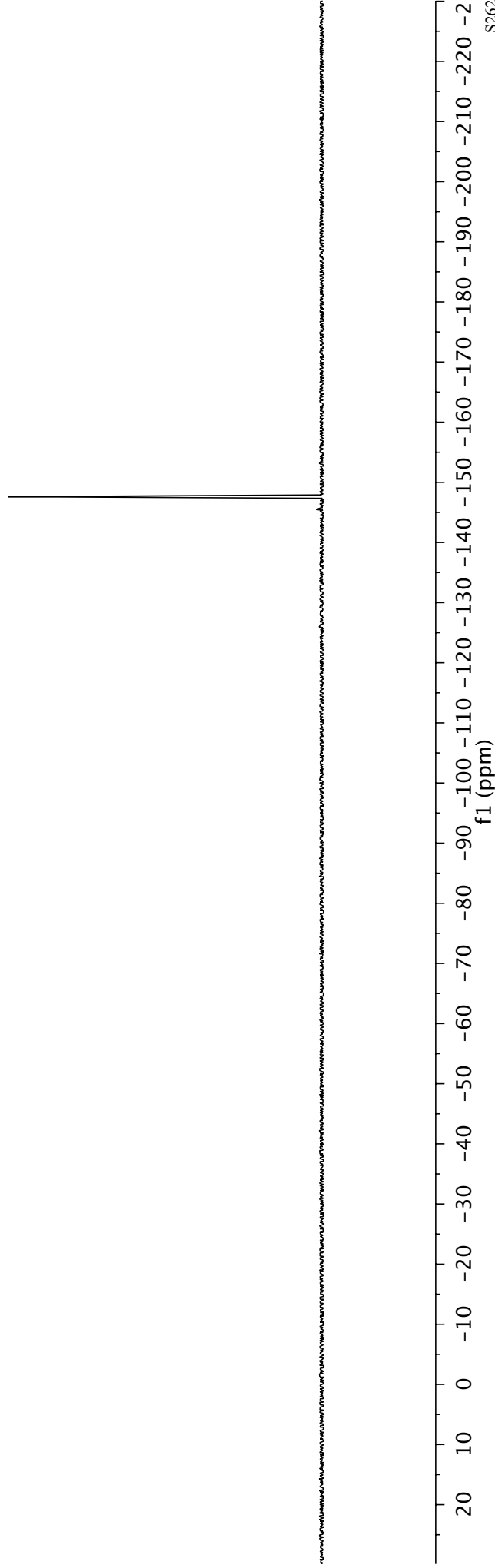
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2200.7
Nucleus	¹³ C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



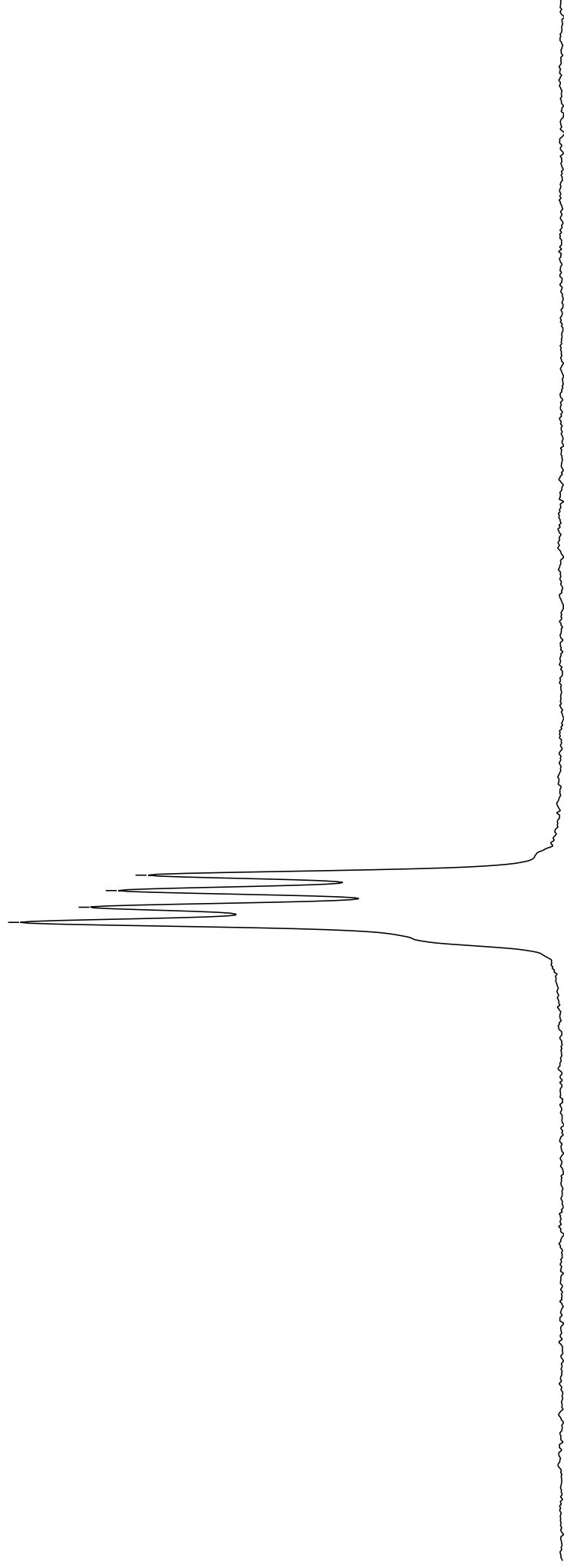
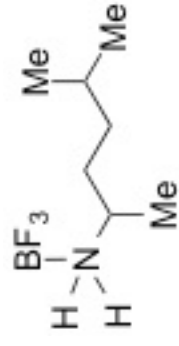




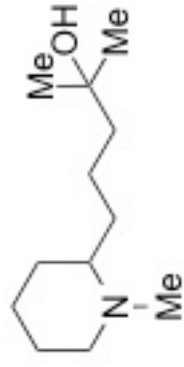
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	56
Relaxation Delay	1.5000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	469.89
Spectral Width	122137.4
Lowest Frequency	-108111.4
Nucleus	19F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



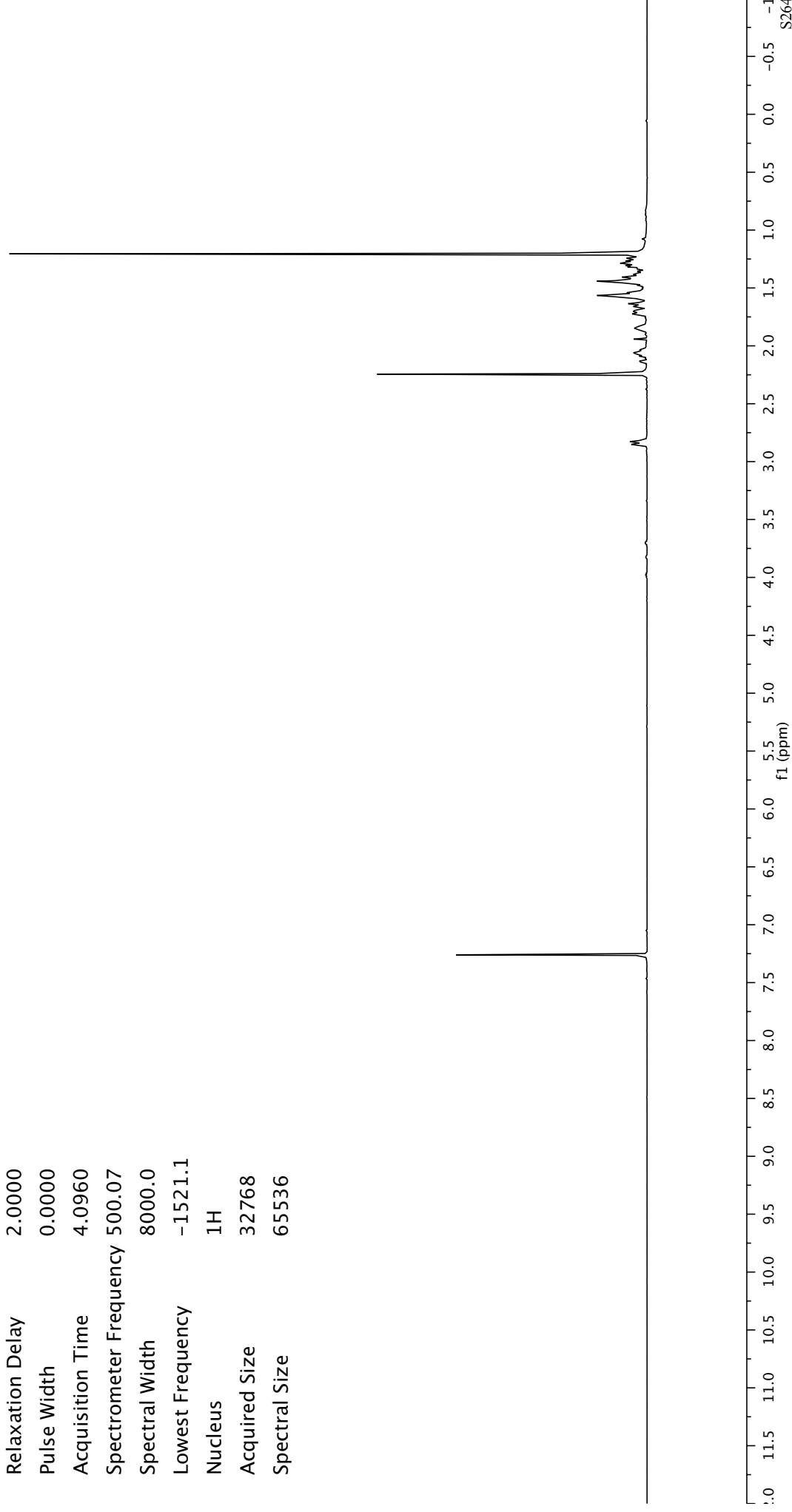
-147.61
-147.65
-147.68
-147.72

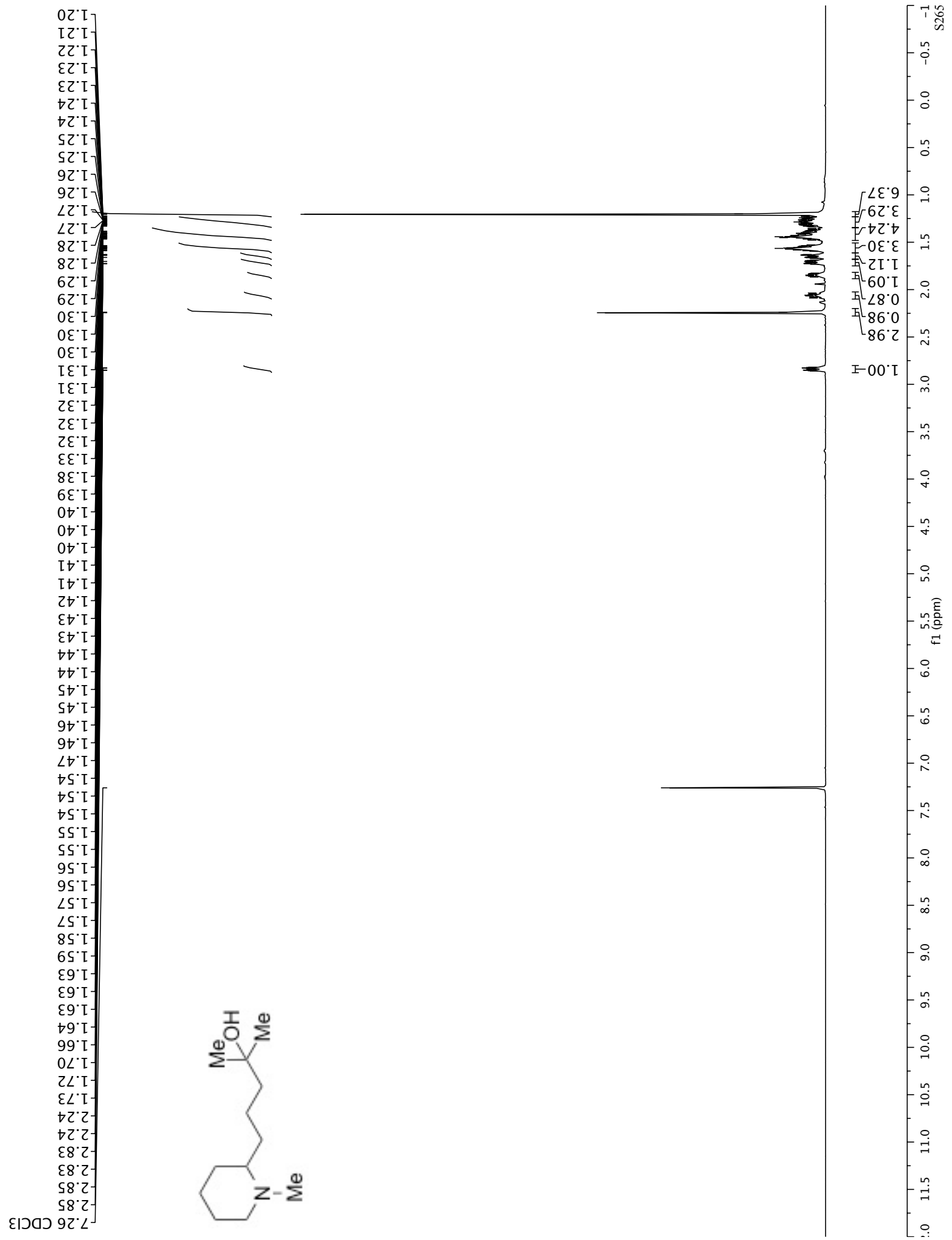


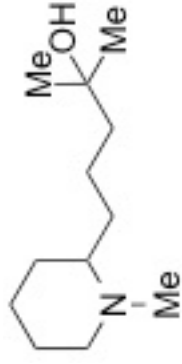
-146.4 -146.6 -146.8 -147.0 -147.2 -147.4 -147.6 -147.8 -148.0 -148.2 -148.4 -148.6 -148.8 -149.0 -149.2 -149.4 -149.6
f1 (ppm)
S263



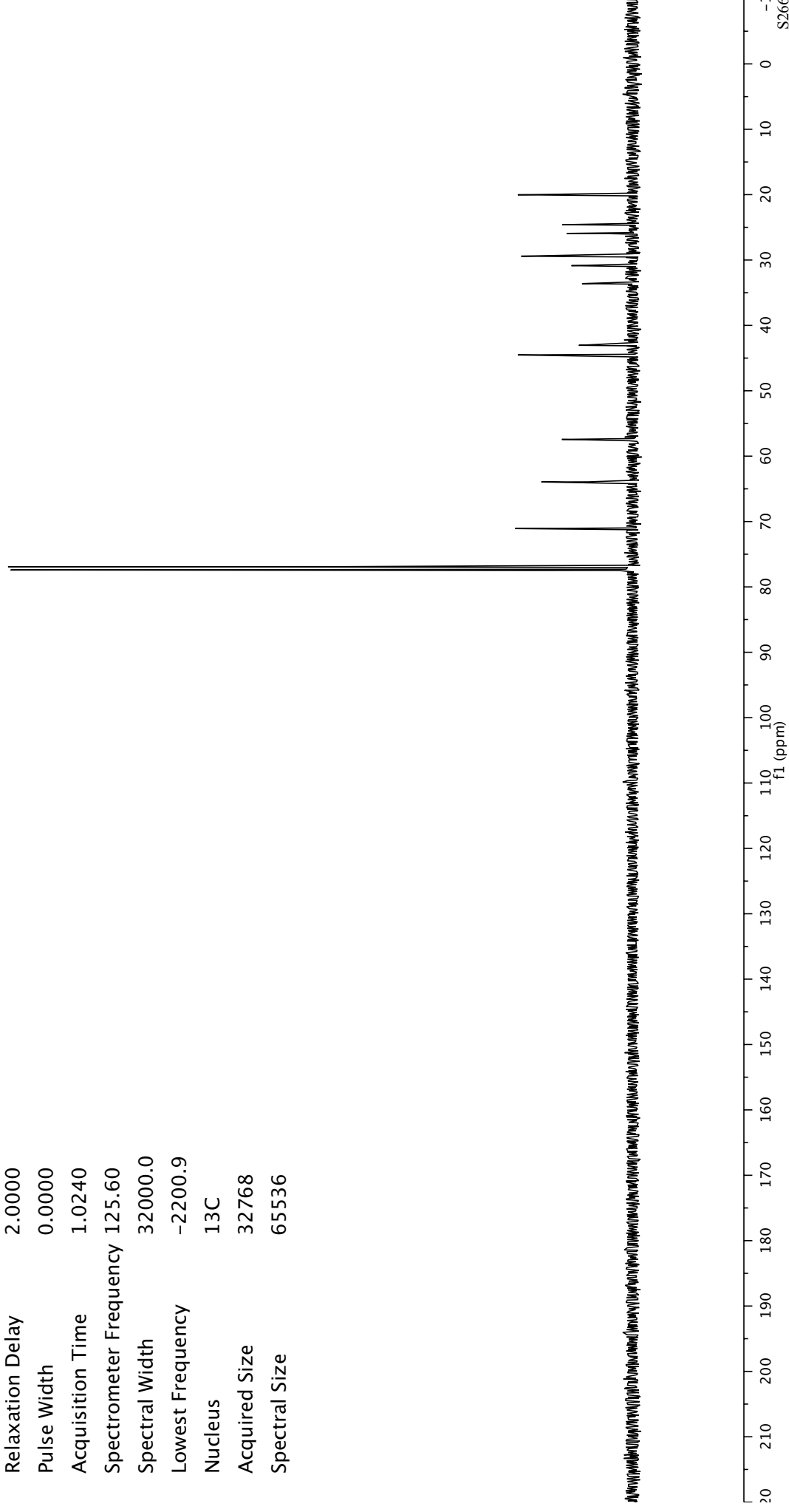
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	28
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1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

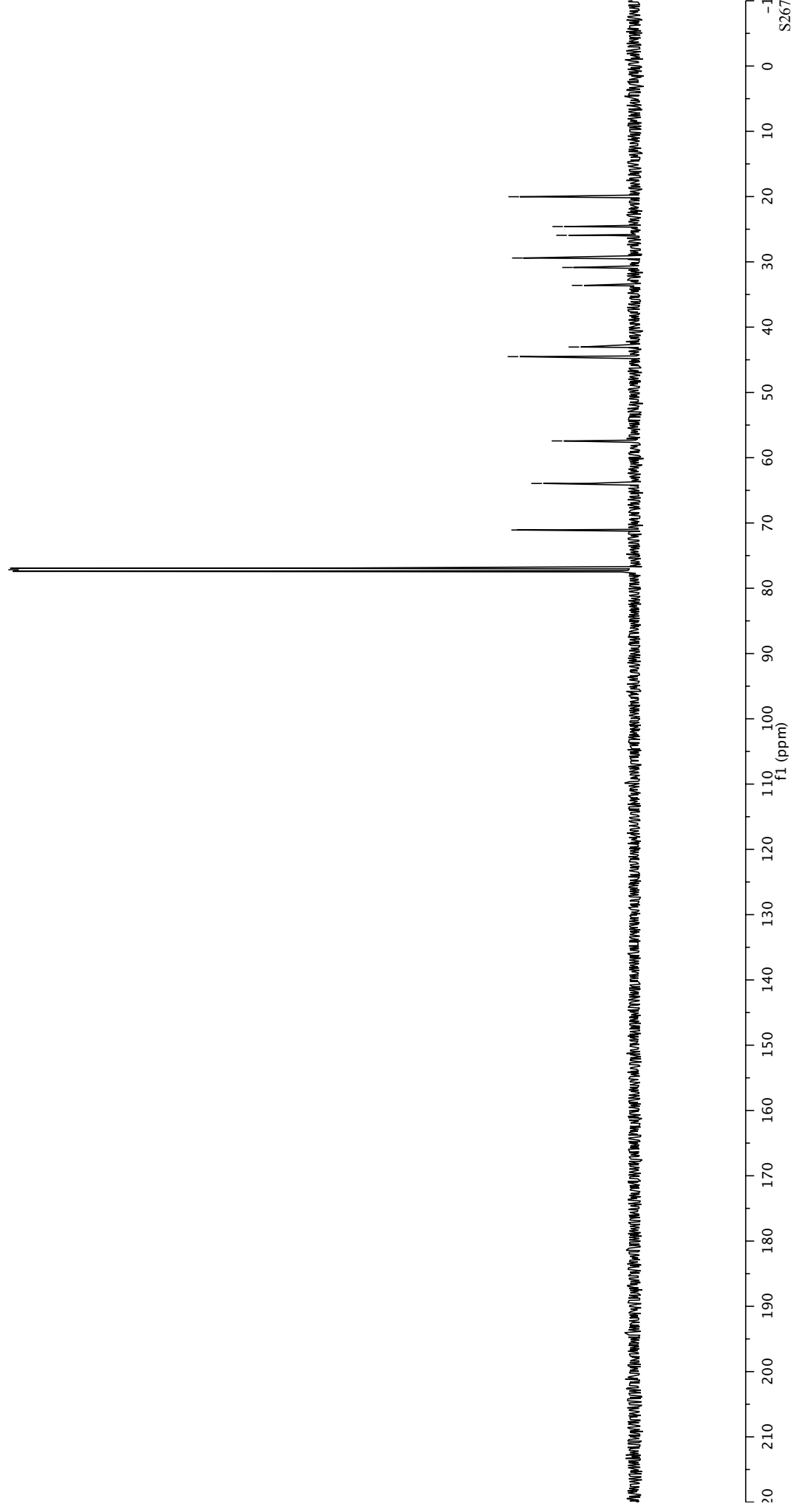
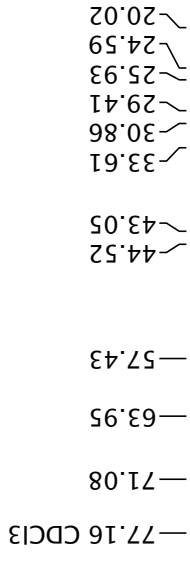
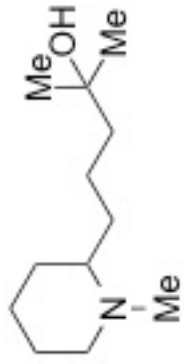


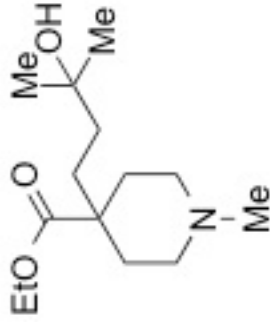




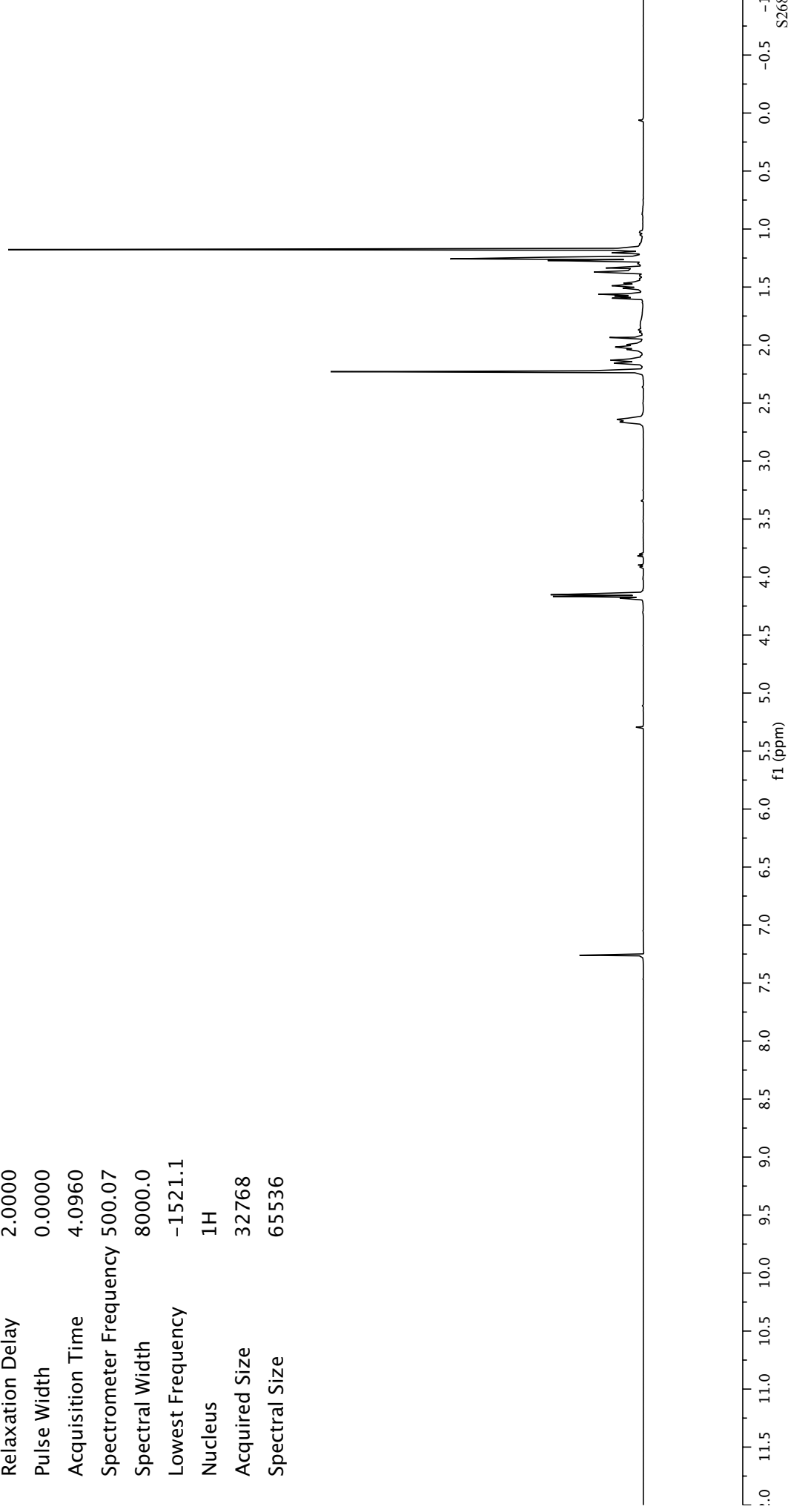
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Number of Scans	653
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2200.9
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

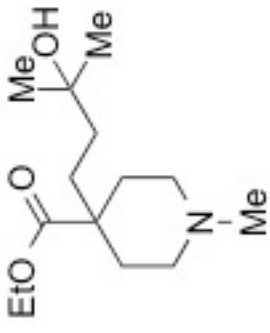




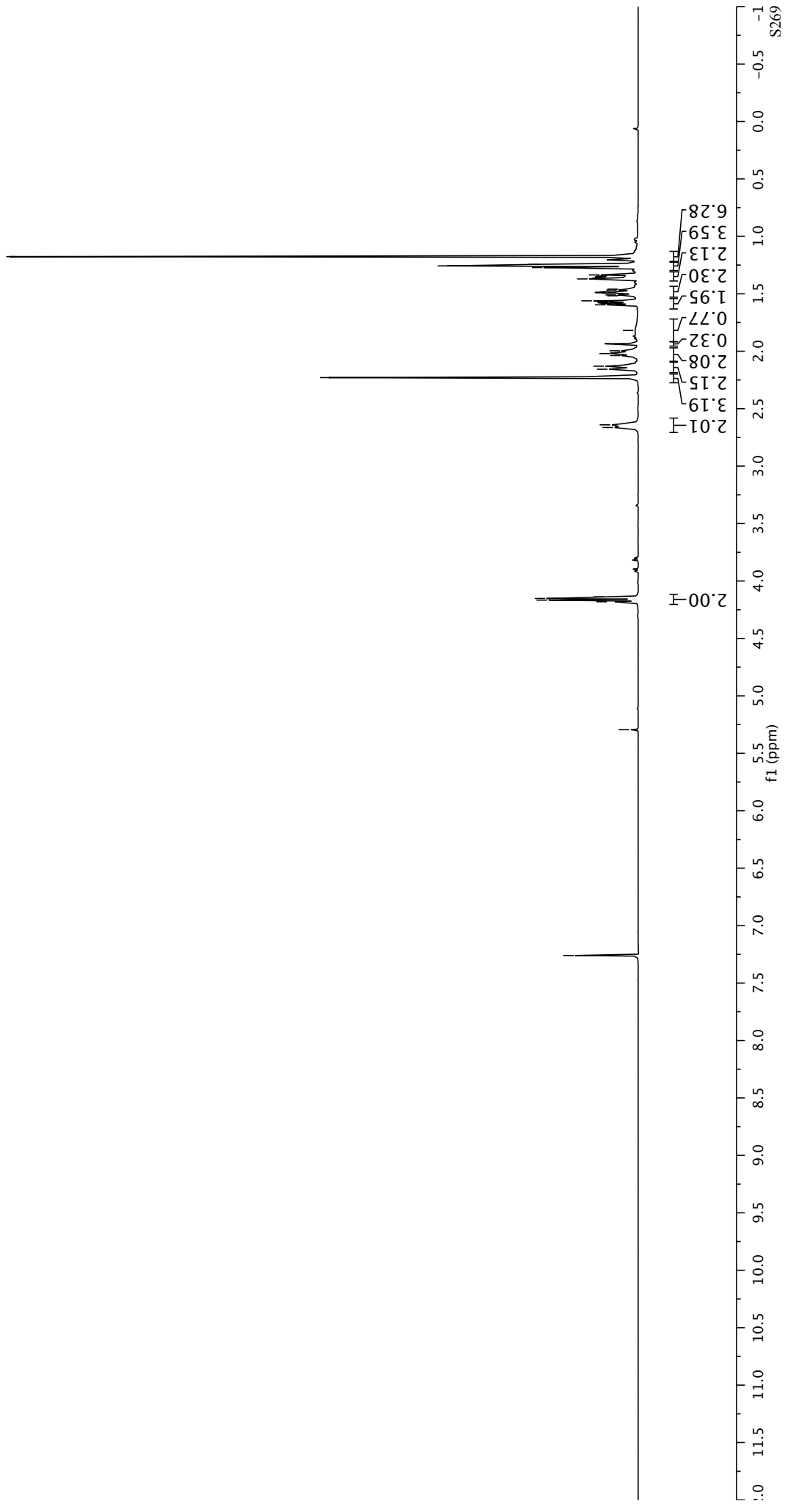
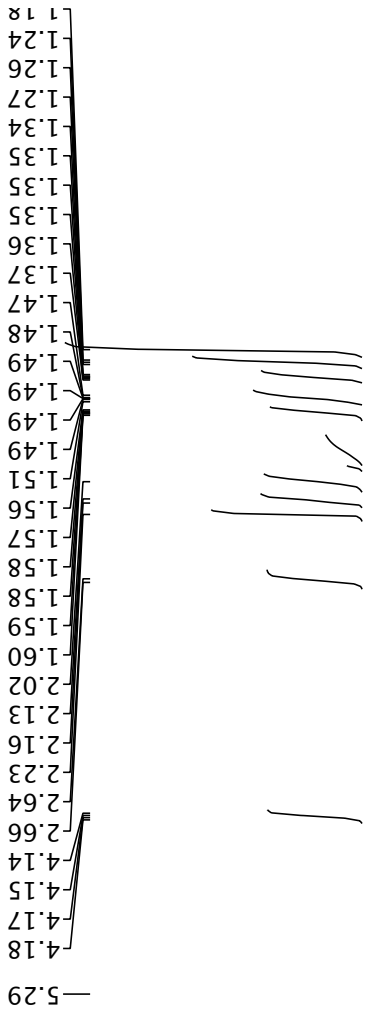


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	34
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1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

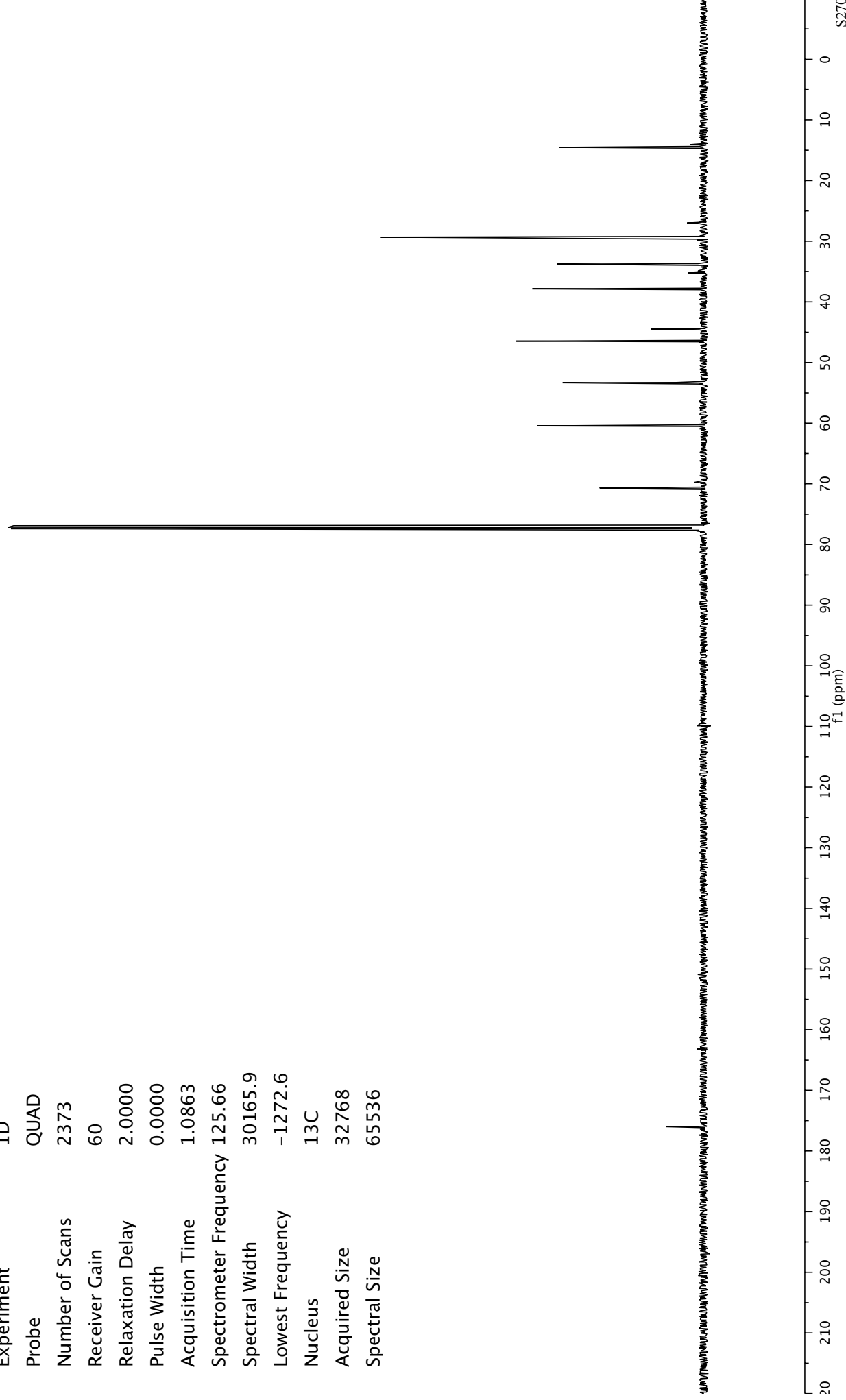
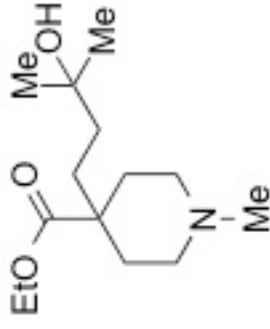


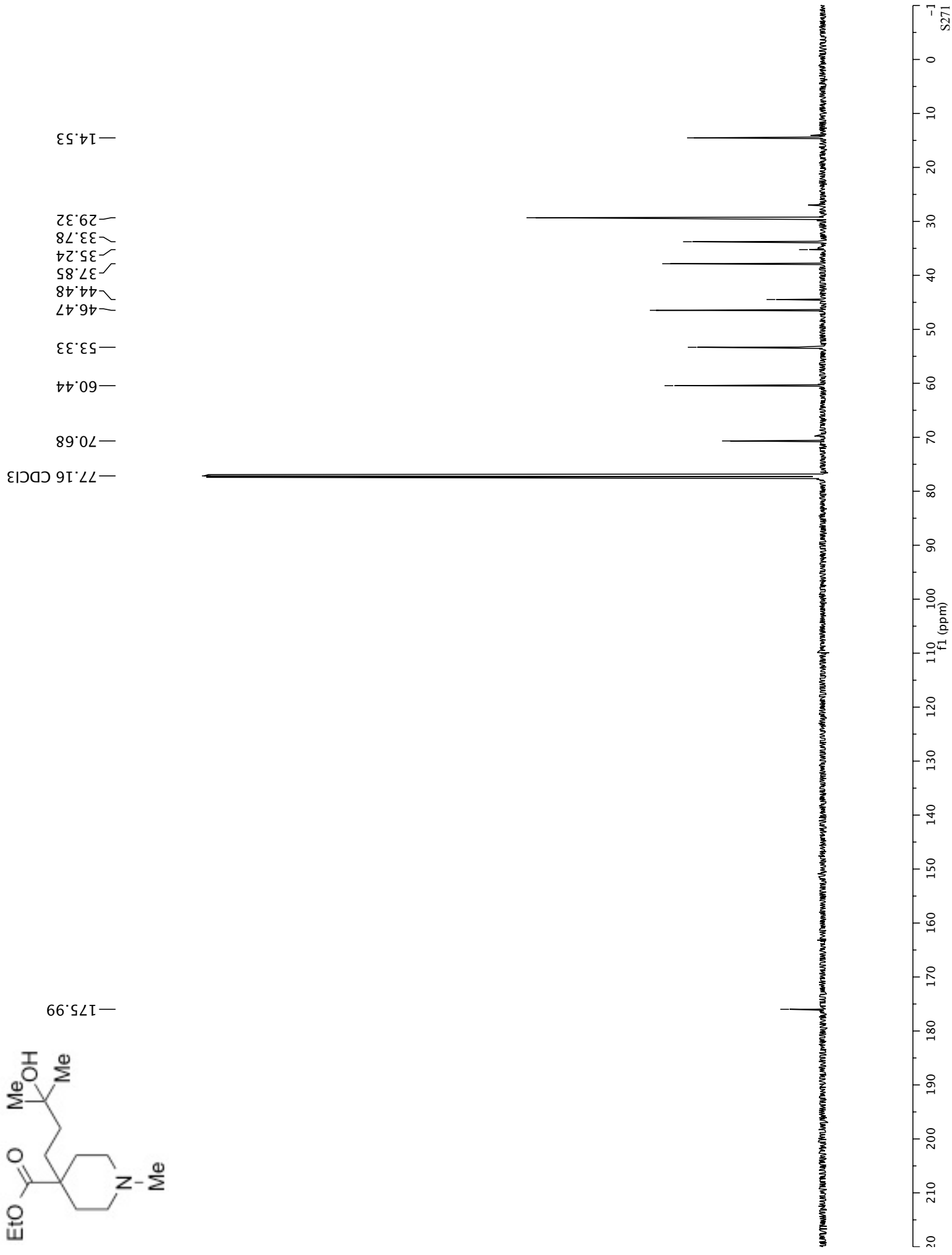
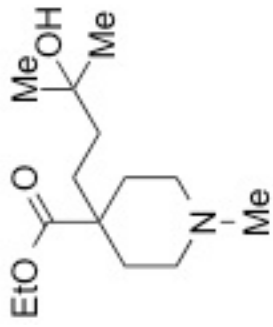


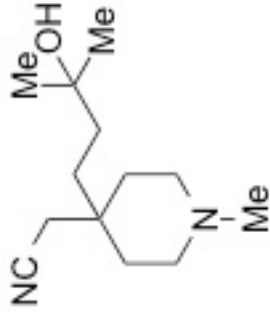
— 7.26 CDCl₃



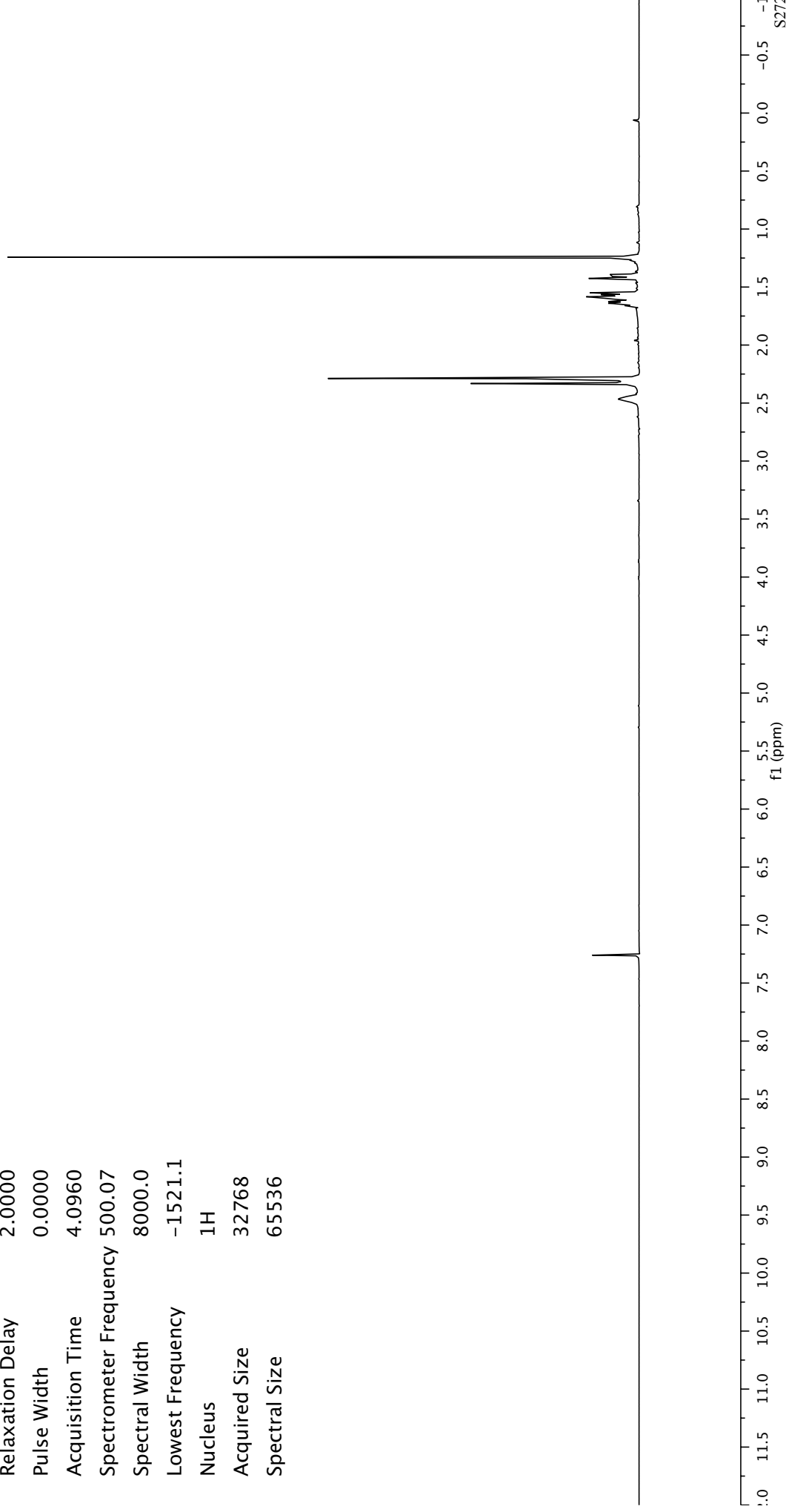
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	2373
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1272.6
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

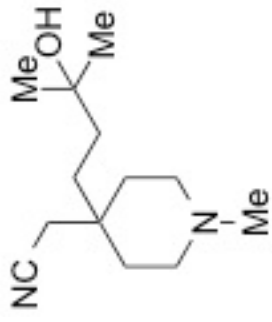




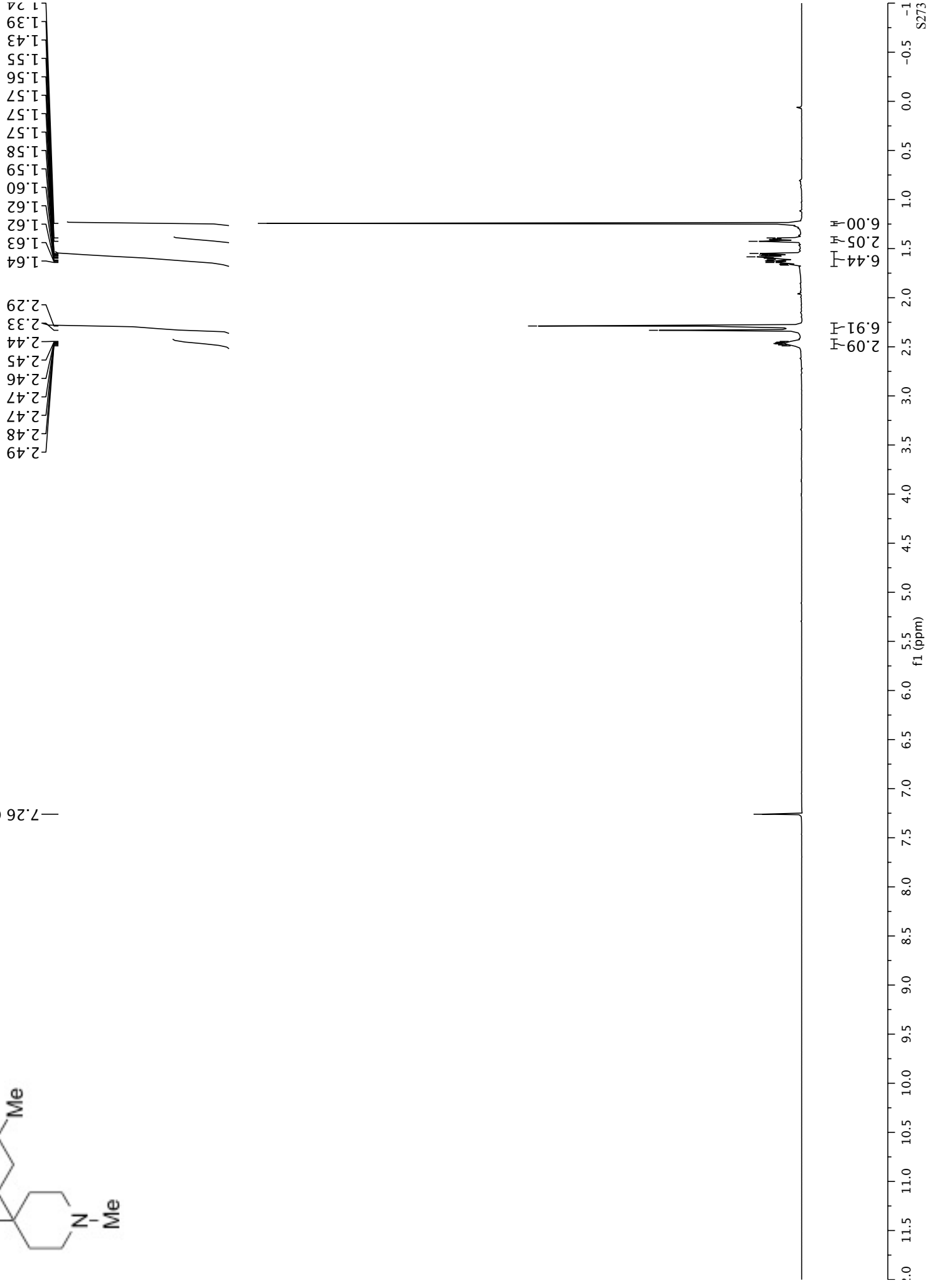


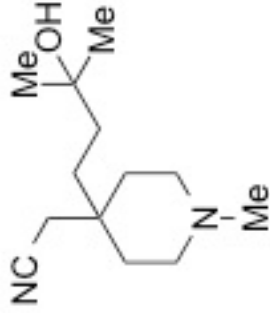
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	32
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1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



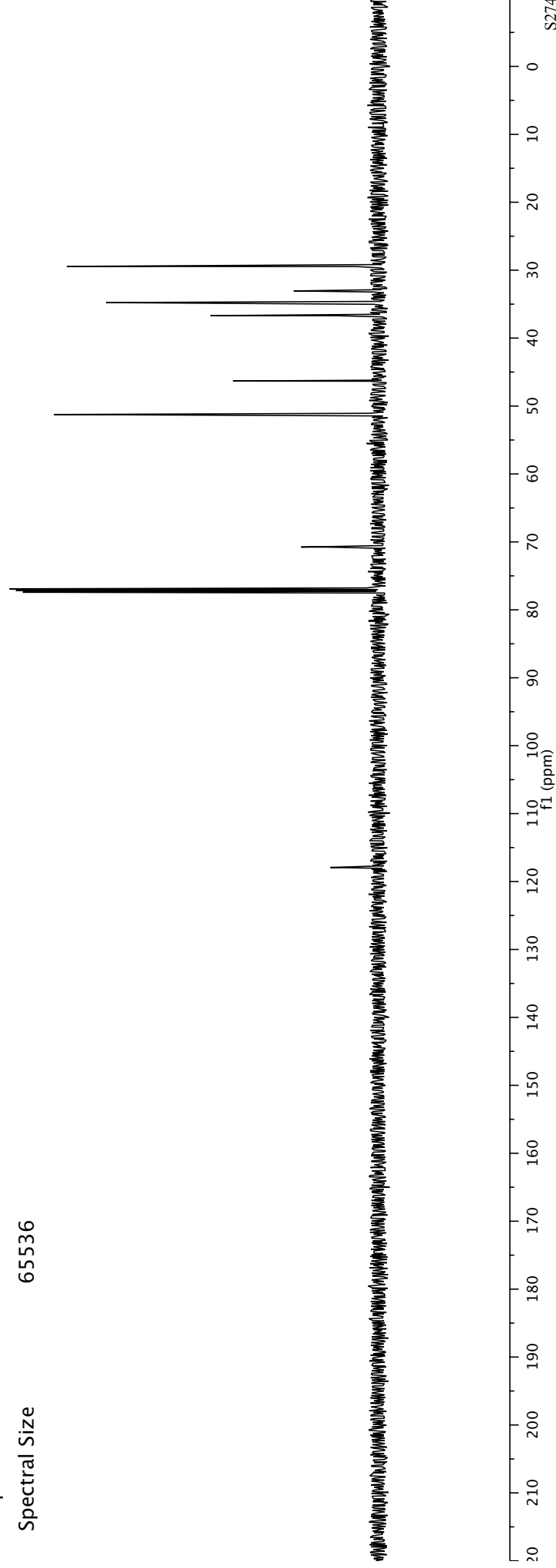


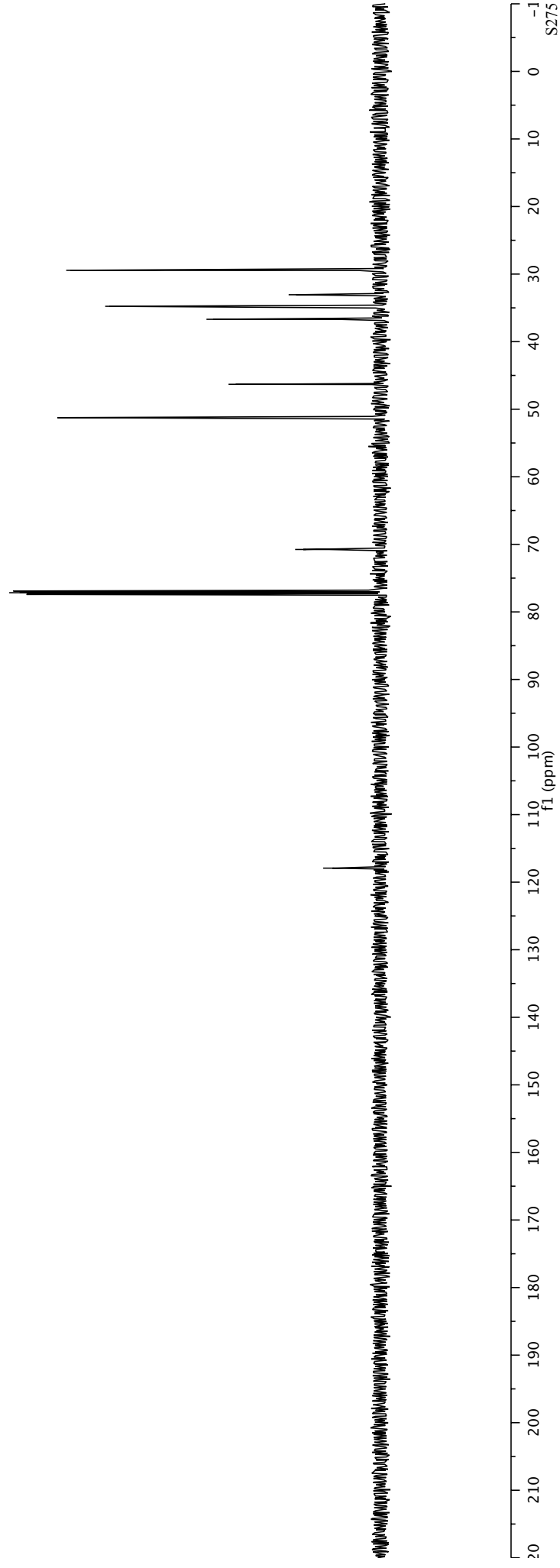
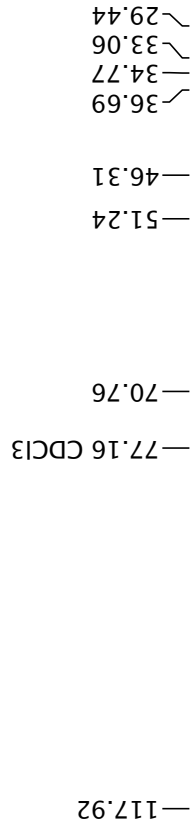
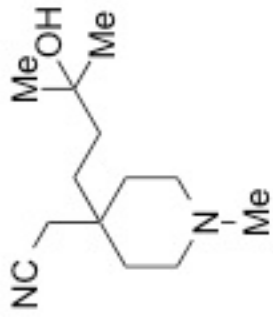
—7.26 CDCl₃

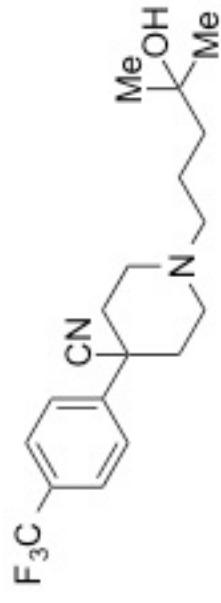




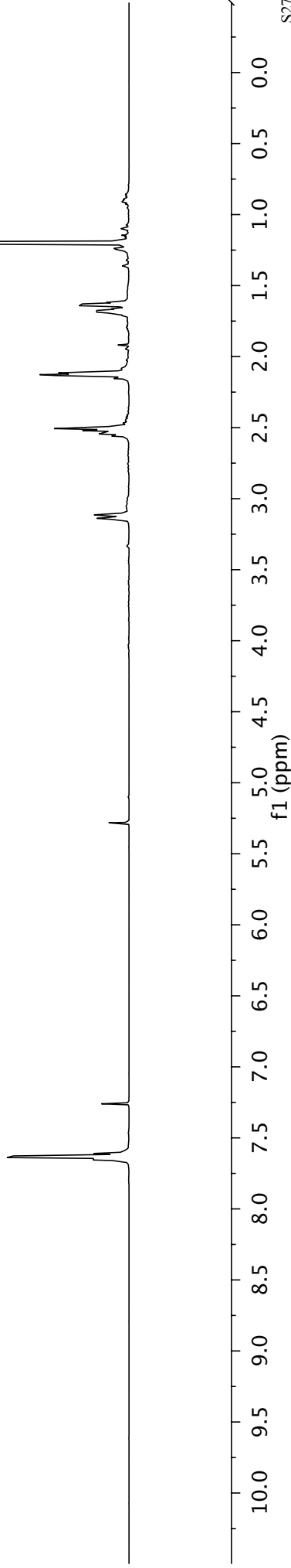
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	662
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1273.1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

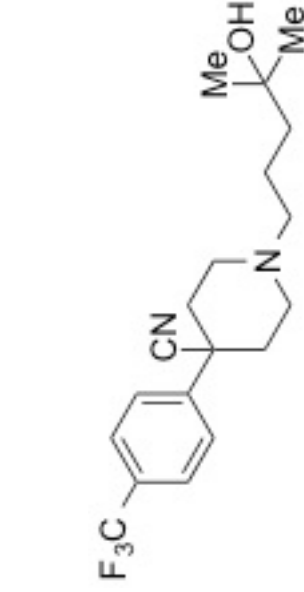






Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	41
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.69
Spectral Width	7024.9
Lowest Frequency	-1021.8
Nucleus	1H
Acquired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



— 5.28 CH₂Cl₂7.26 CDCl₃
7.61
7.63
7.64
7.663.14
3.11
2.56
2.54
2.53
2.52
2.51
2.50
2.13
2.13
2.12
2.11
1.71
1.70
1.69
1.67
1.66
1.64
1.63
1.62
1.20
0.91

DCM

2.25
2.20

2.00

4.11

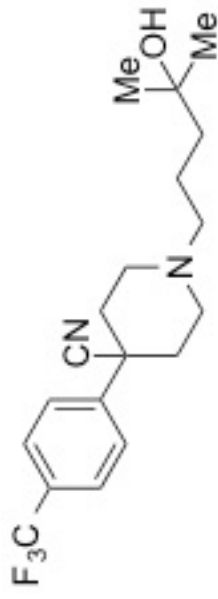
4.49

3.98

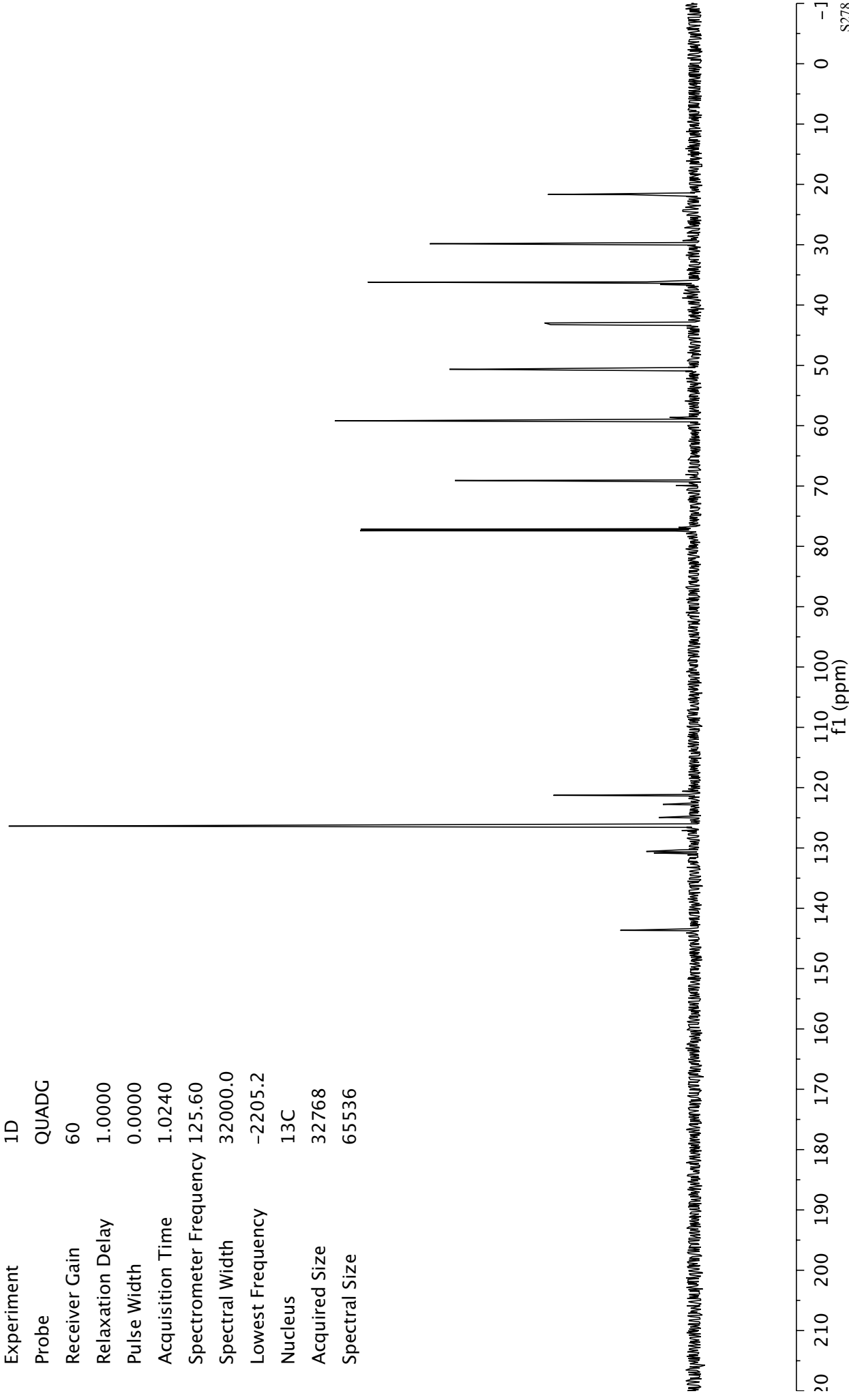
0.23

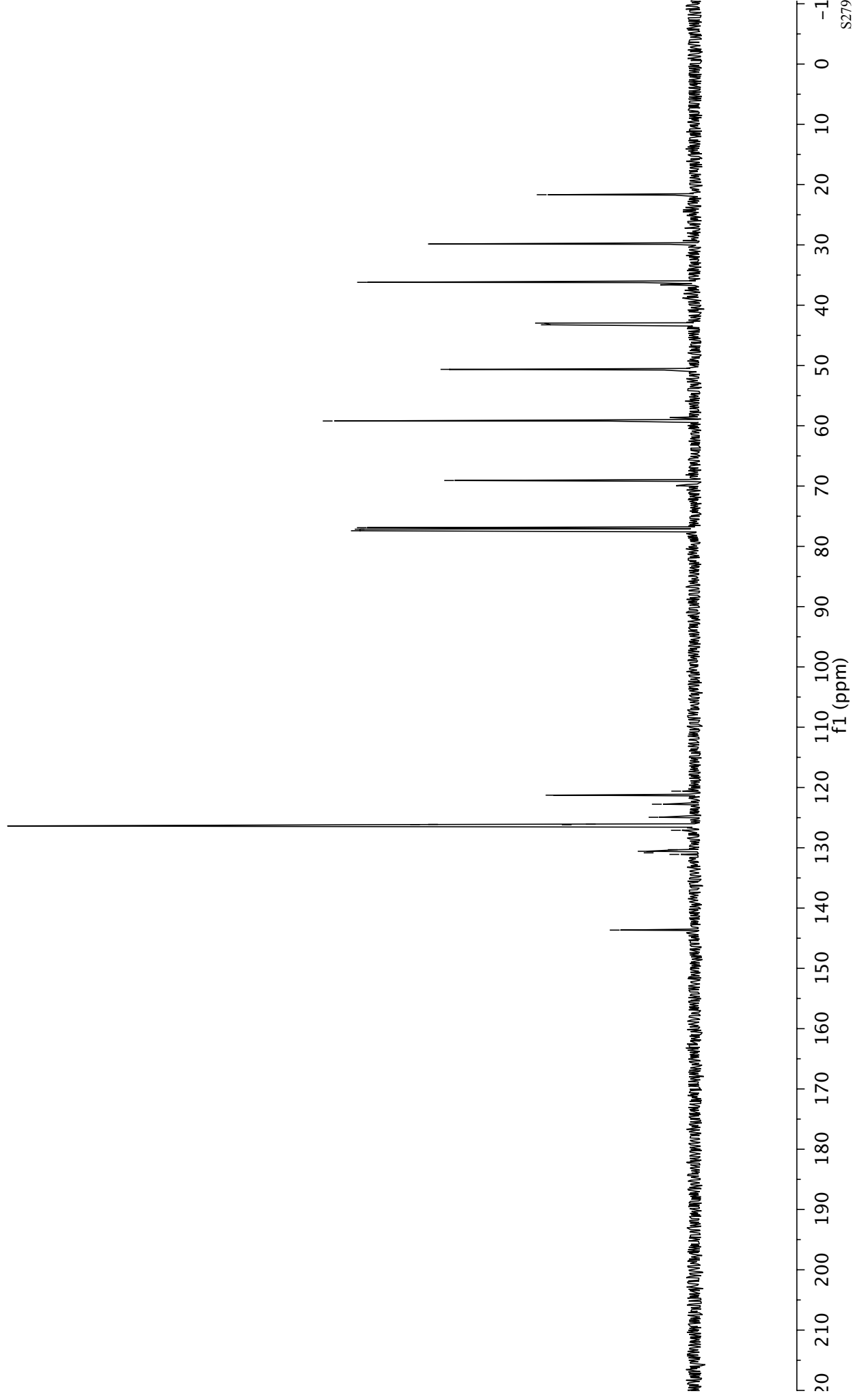
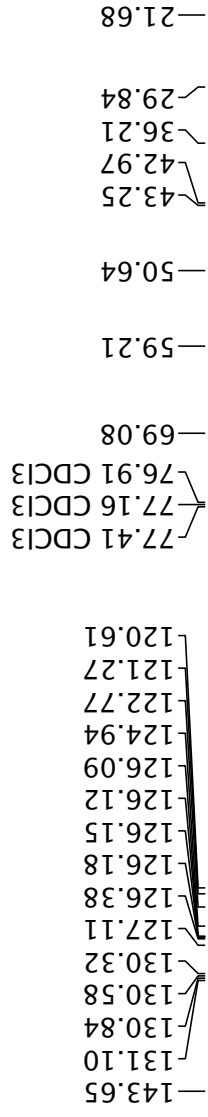
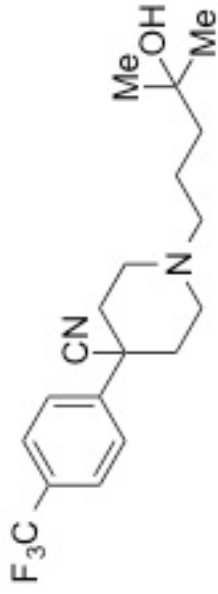
5.99

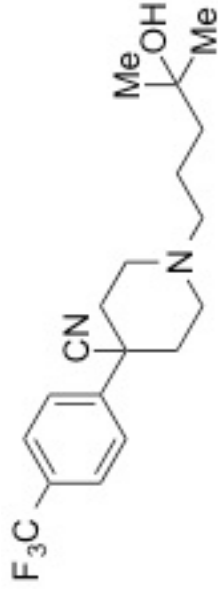
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)



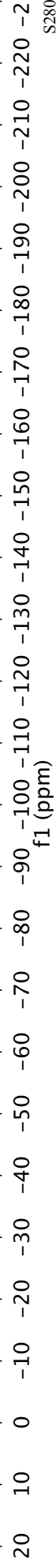
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2205.2
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

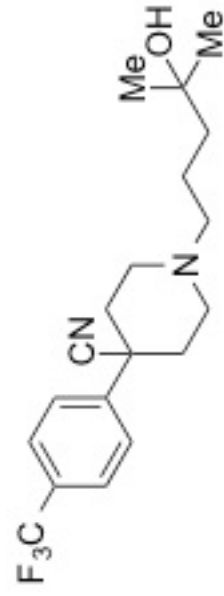






Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	56
Relaxation Delay	1.5000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	469.89
Spectral Width	122137.4
Lowest Frequency	-108111.4
Nucleus	¹⁹ F
Acquired Size	40022
Spectral Size	131072





63.24

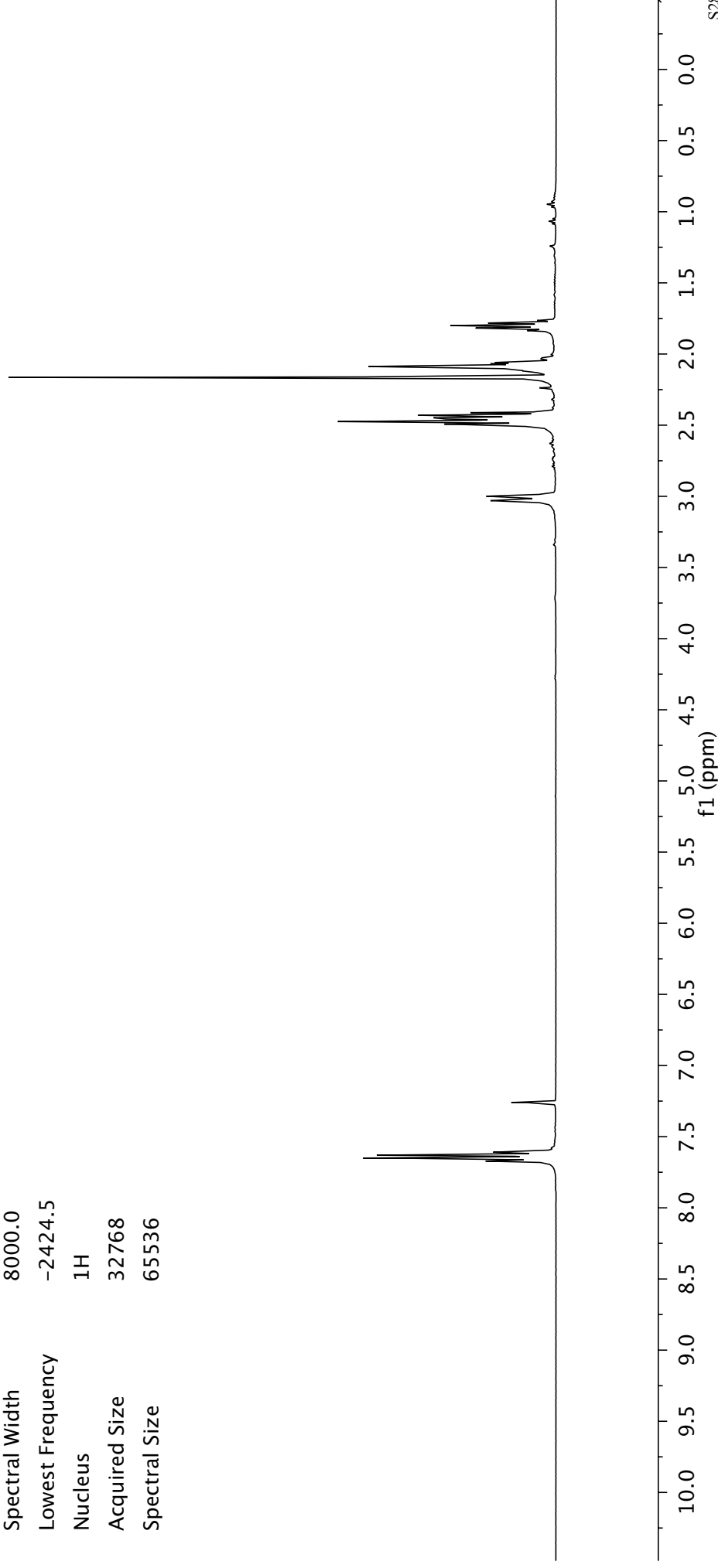
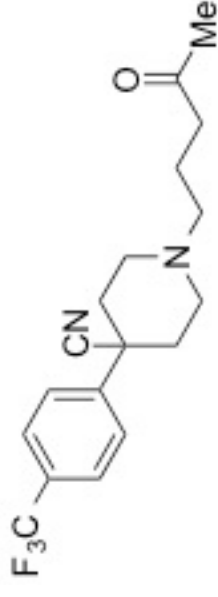
3.00

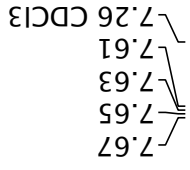
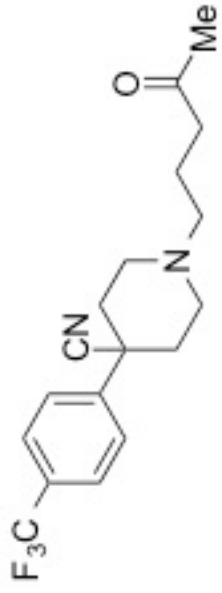
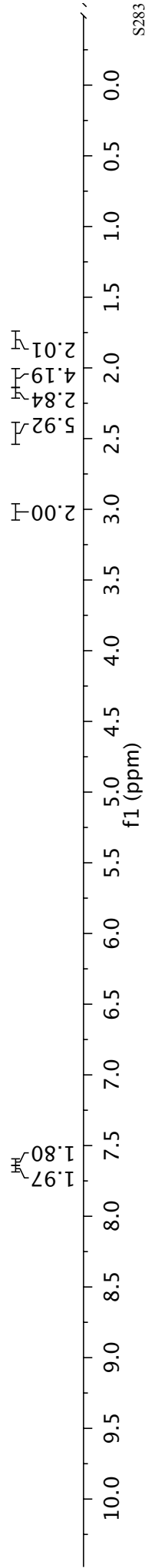
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -2

f1 (ppm)

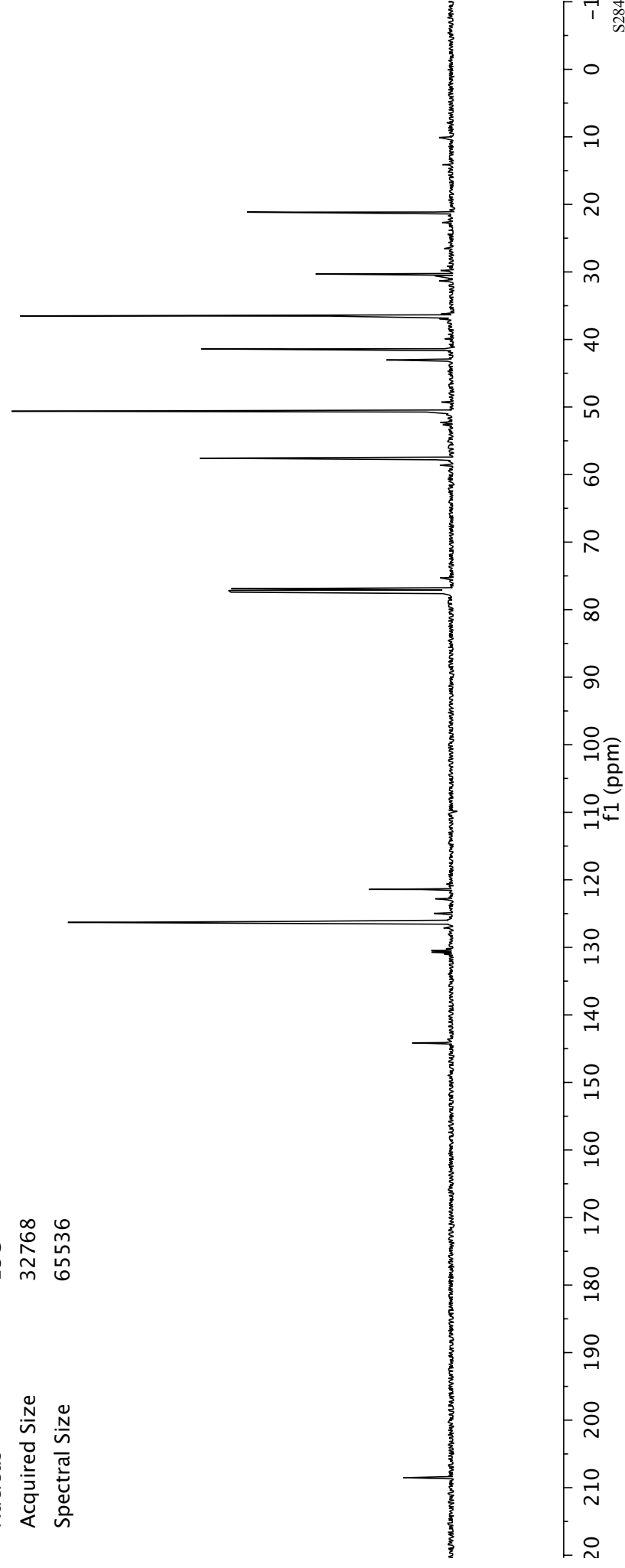
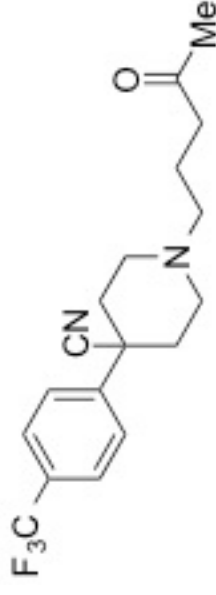
S281

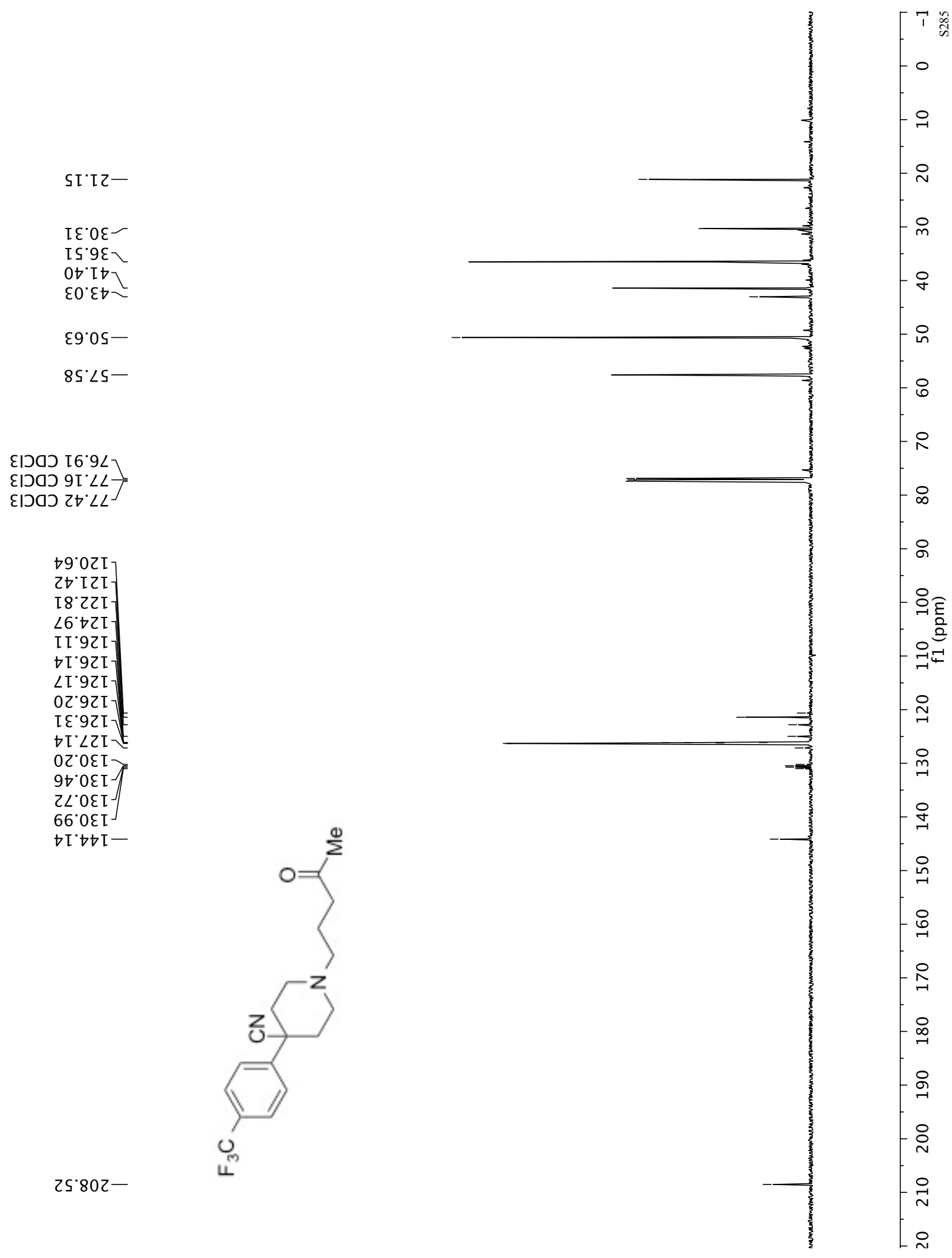
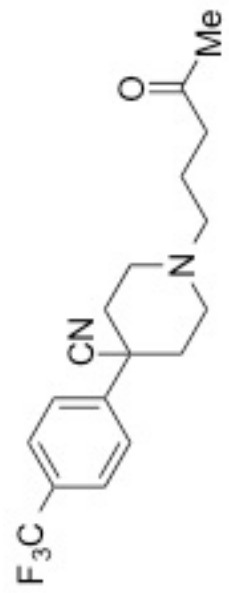
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	46
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	399.95
Spectral Width	8000.0
Lowest Frequency	-2424.5
Nucleus	¹ H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

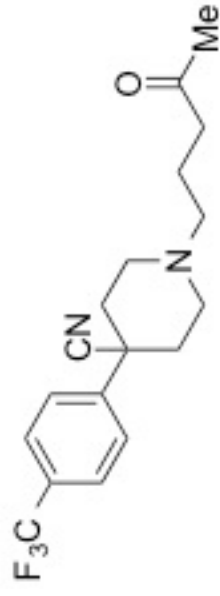




Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1275.8
Nucleus	13C
Acquired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

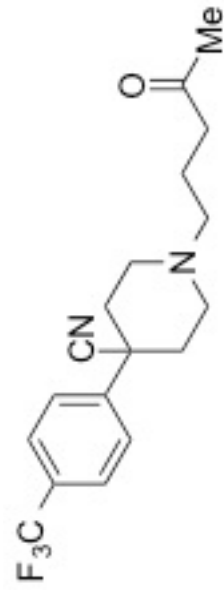






Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	50
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency	-79541.0
Nucleus	19F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



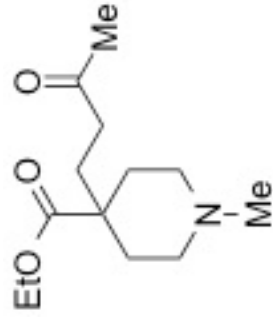


-63.21

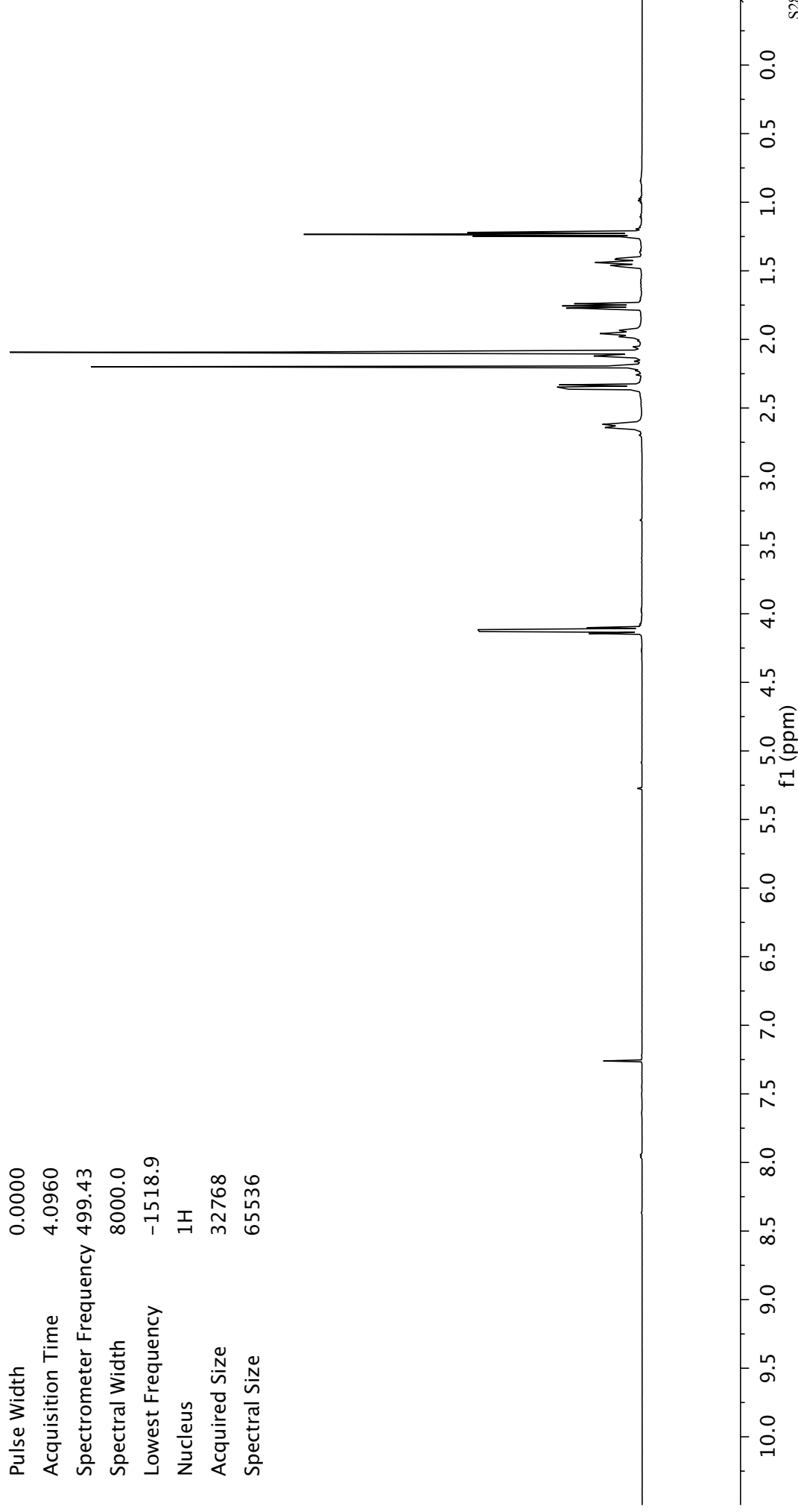
3.00
f1 (ppm)

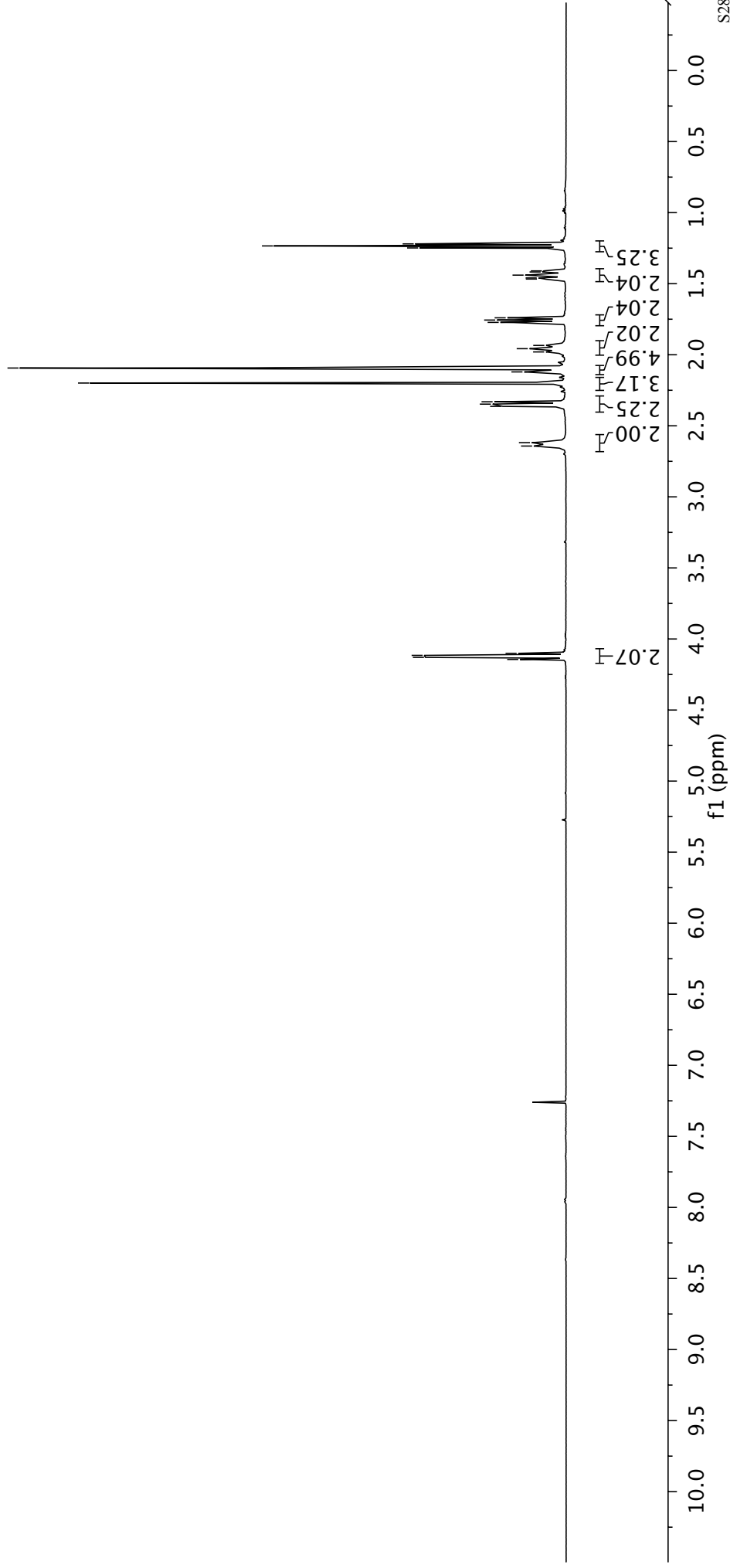
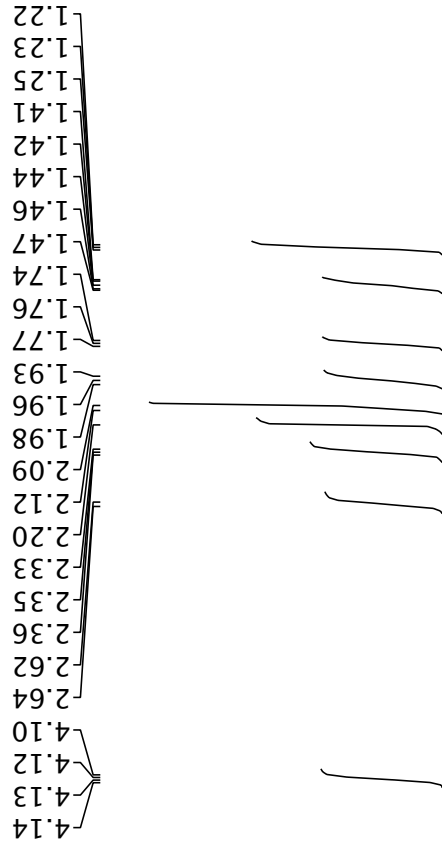
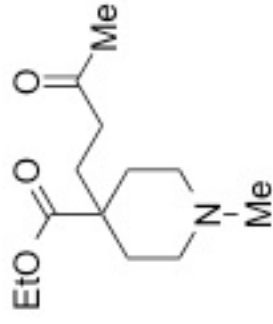
-60 -50 -40 -30 -20 -10 0 10 20 30 40

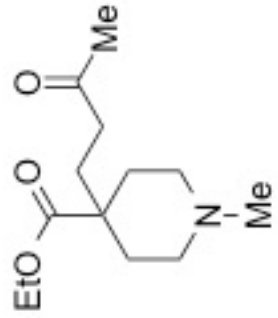
-160 -150 -140 -130 -120 -110 -100 -90 -80 -70 -60



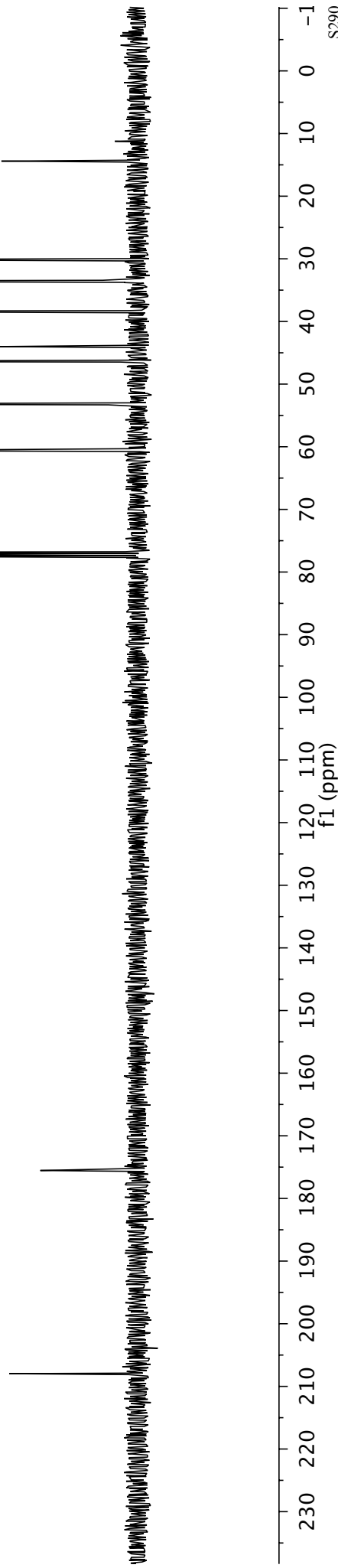
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	44
Relaxation Delay	5.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	499.43
Spectral Width	8000.0
Lowest Frequency	-1518.9
Nucleus	¹ H
Acquired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

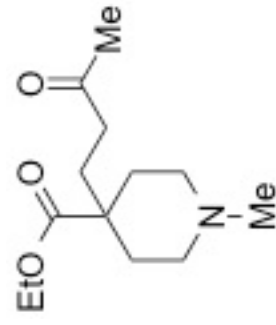






Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.3107
Spectrometer Frequency	100.58
Spectral Width	25000.0
Lowest Frequency	-1028.1
Nucleus	¹³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

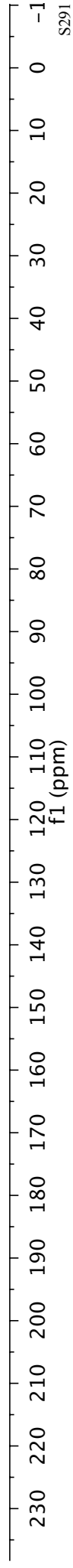
38.36

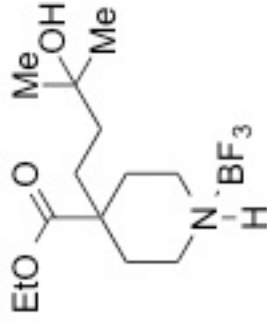
33.57

30.12

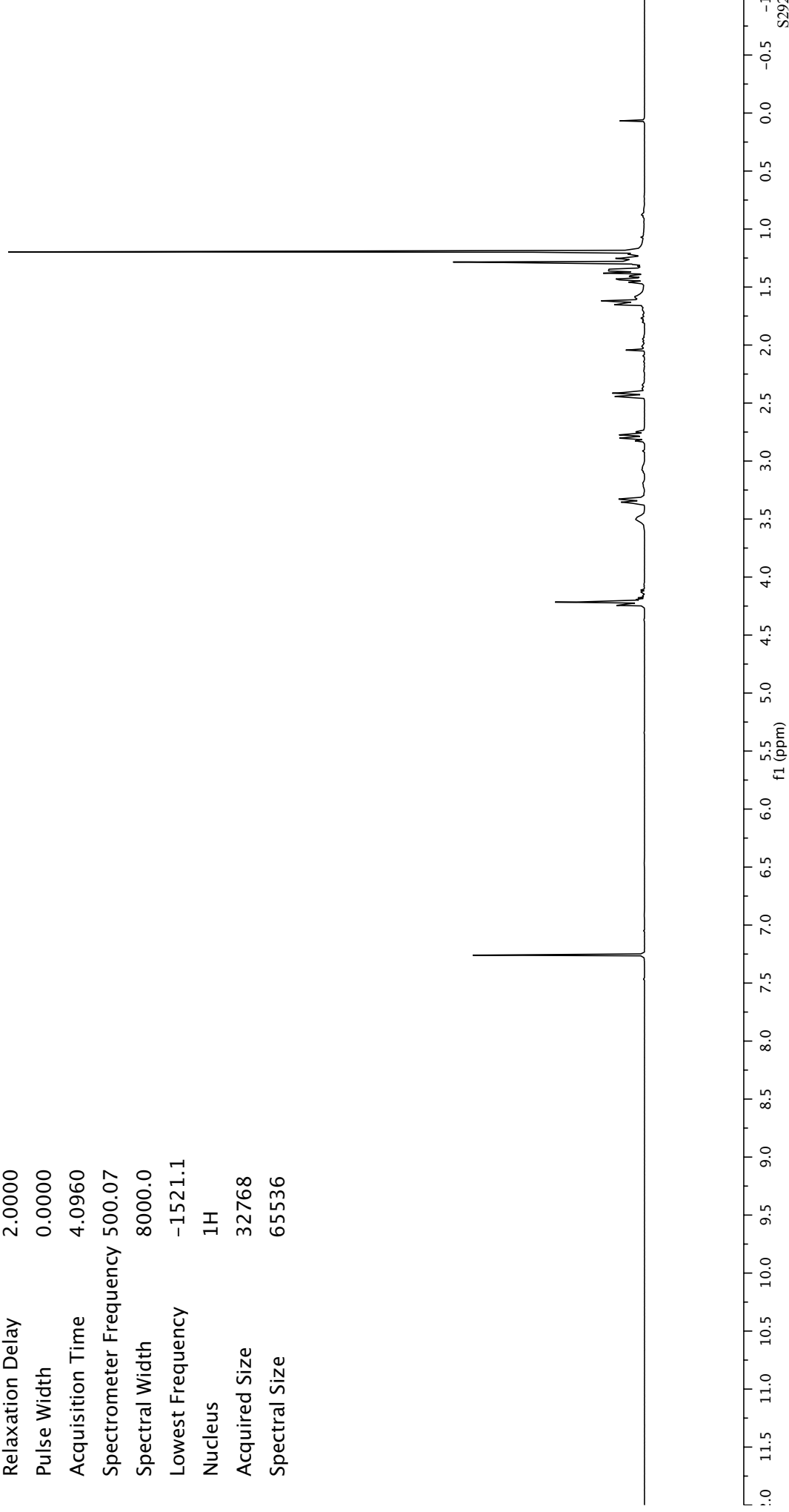
14.40

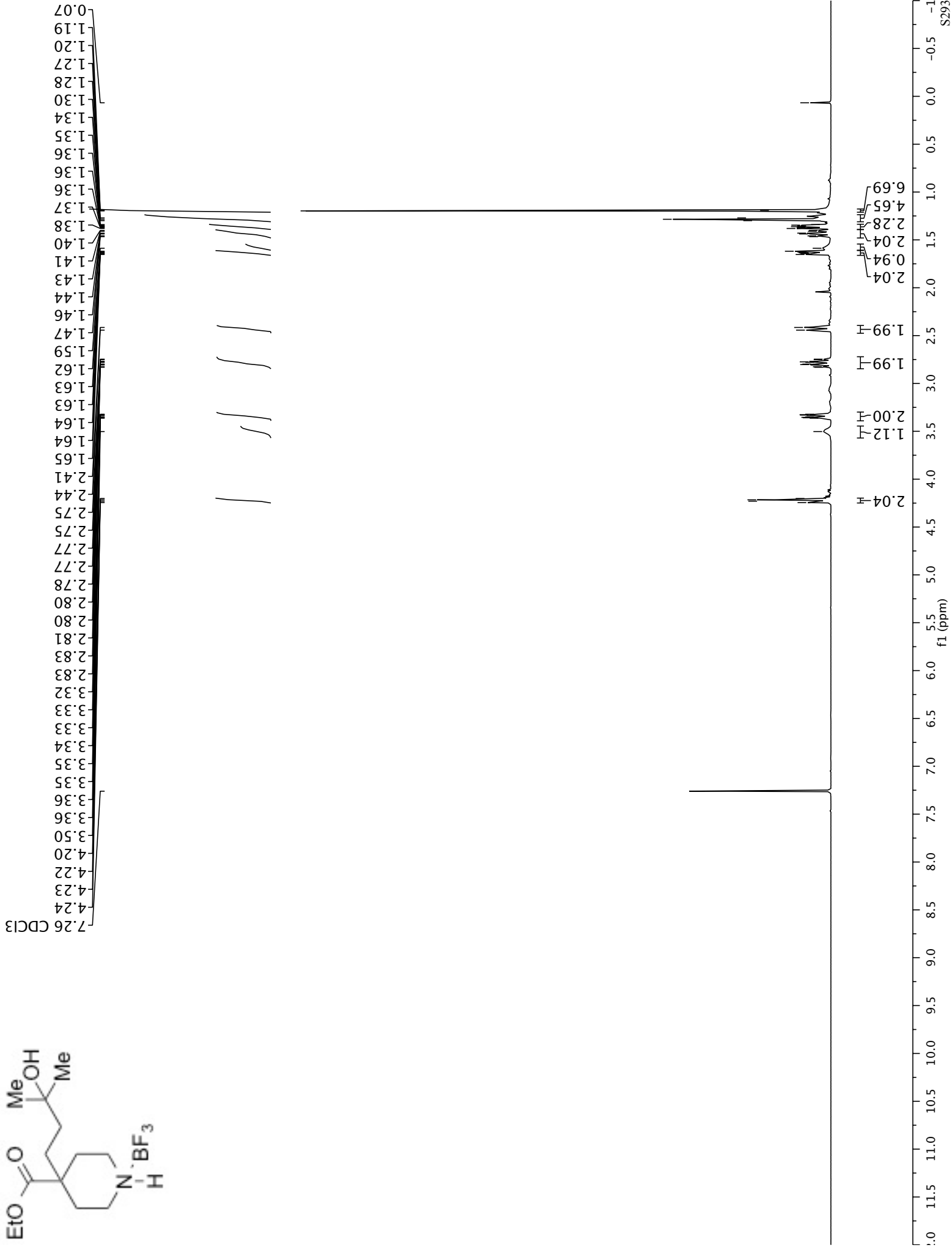
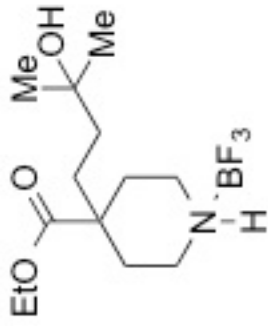
14.38

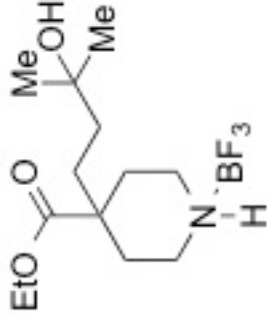




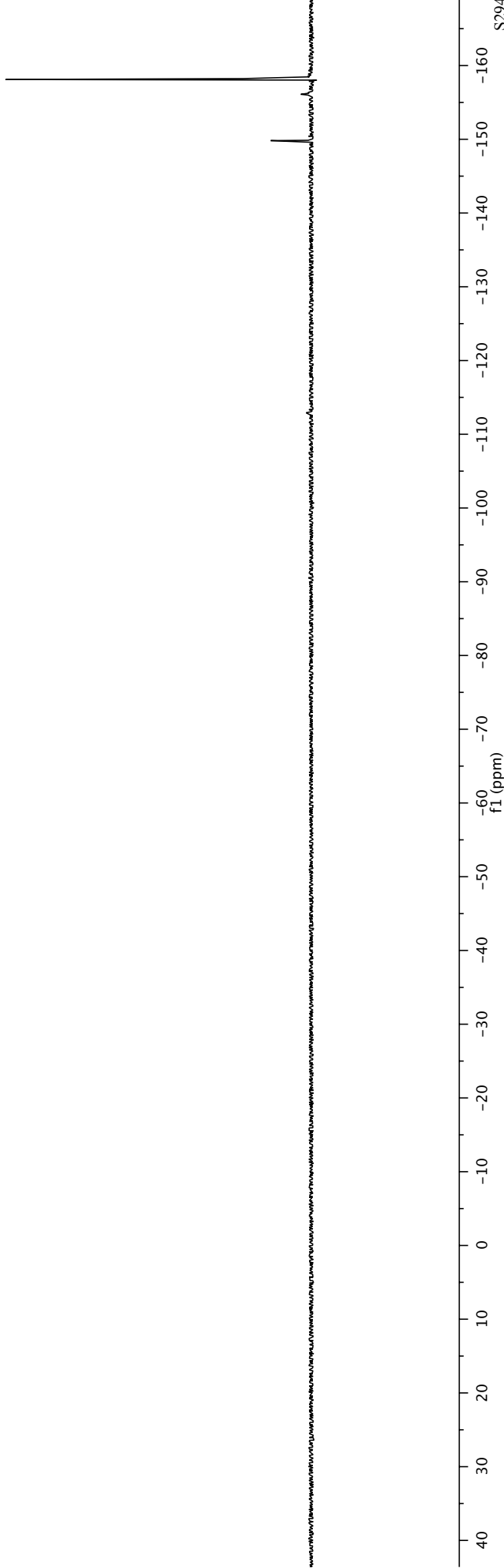
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	44
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

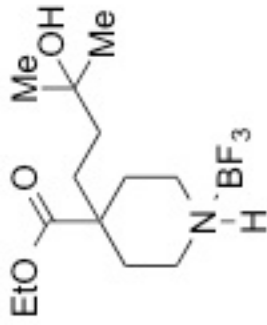




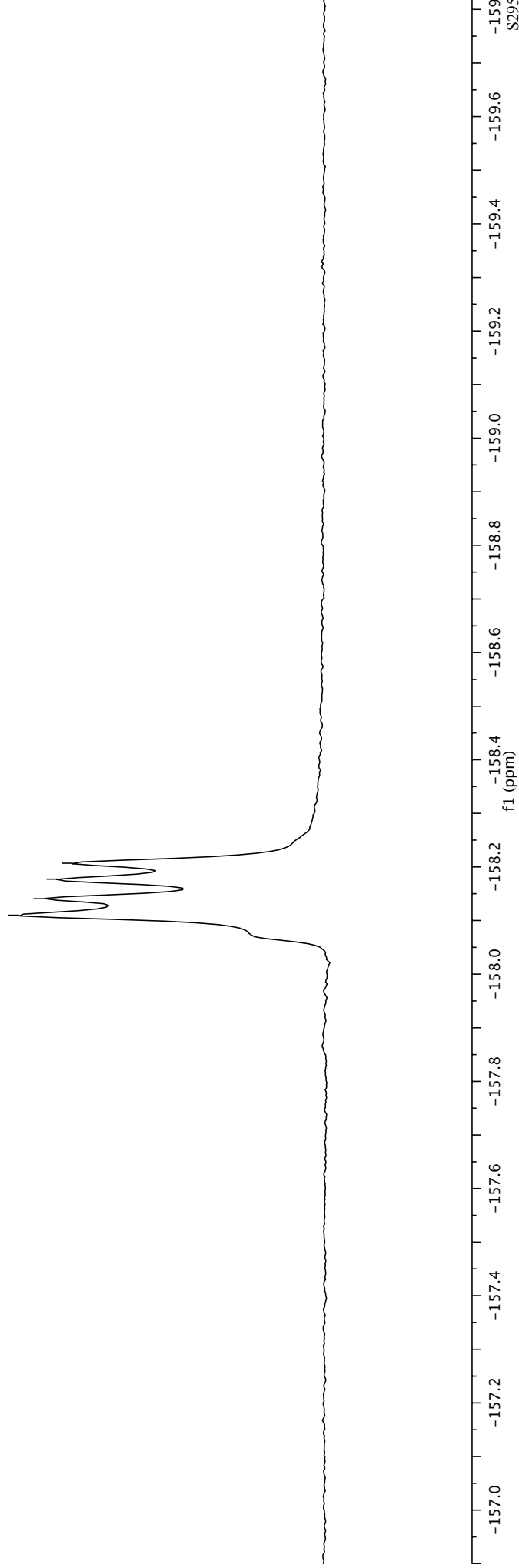


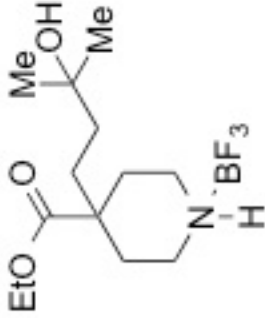
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	22.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	64
Receiver Gain	50
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency	-79501.3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



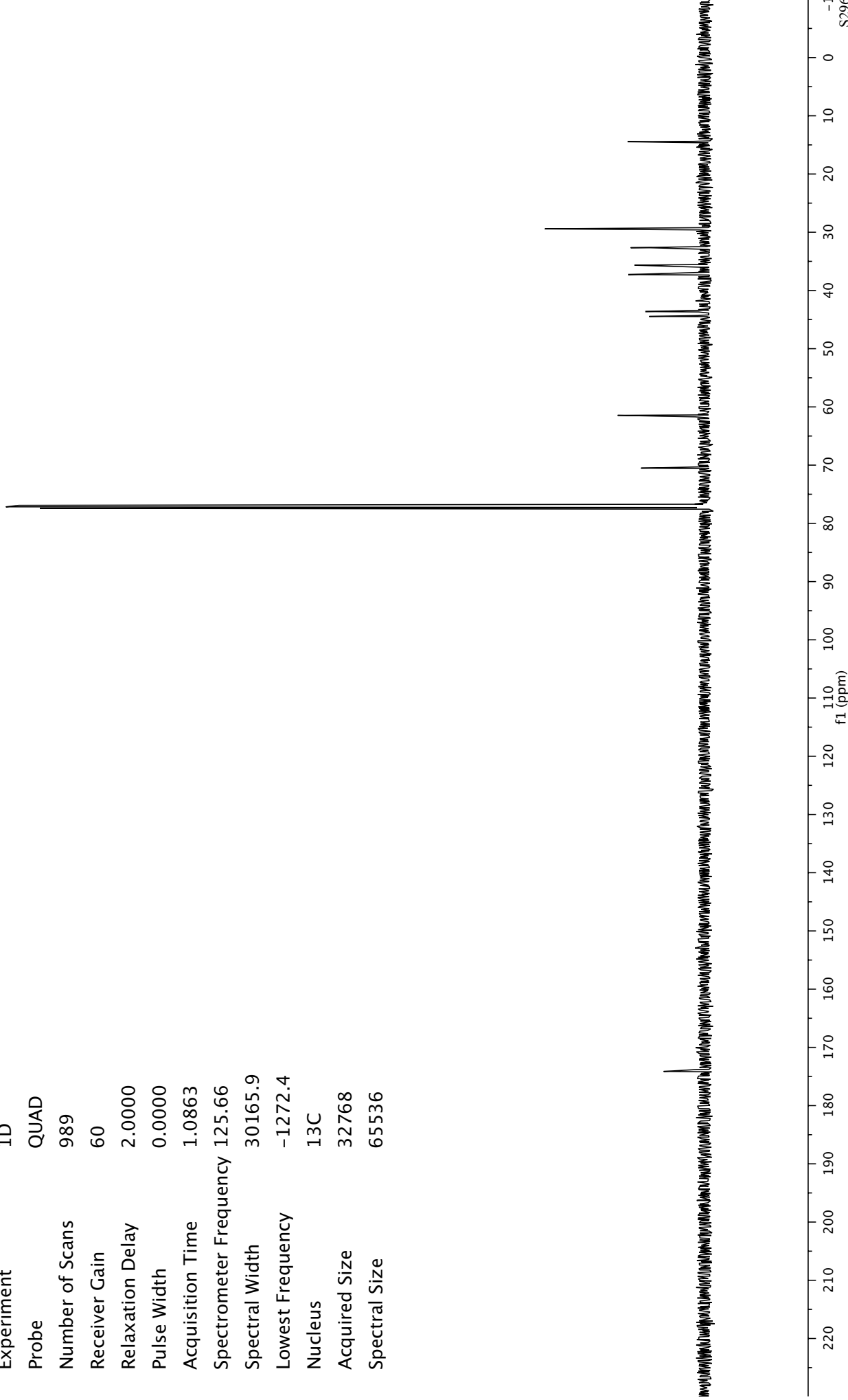


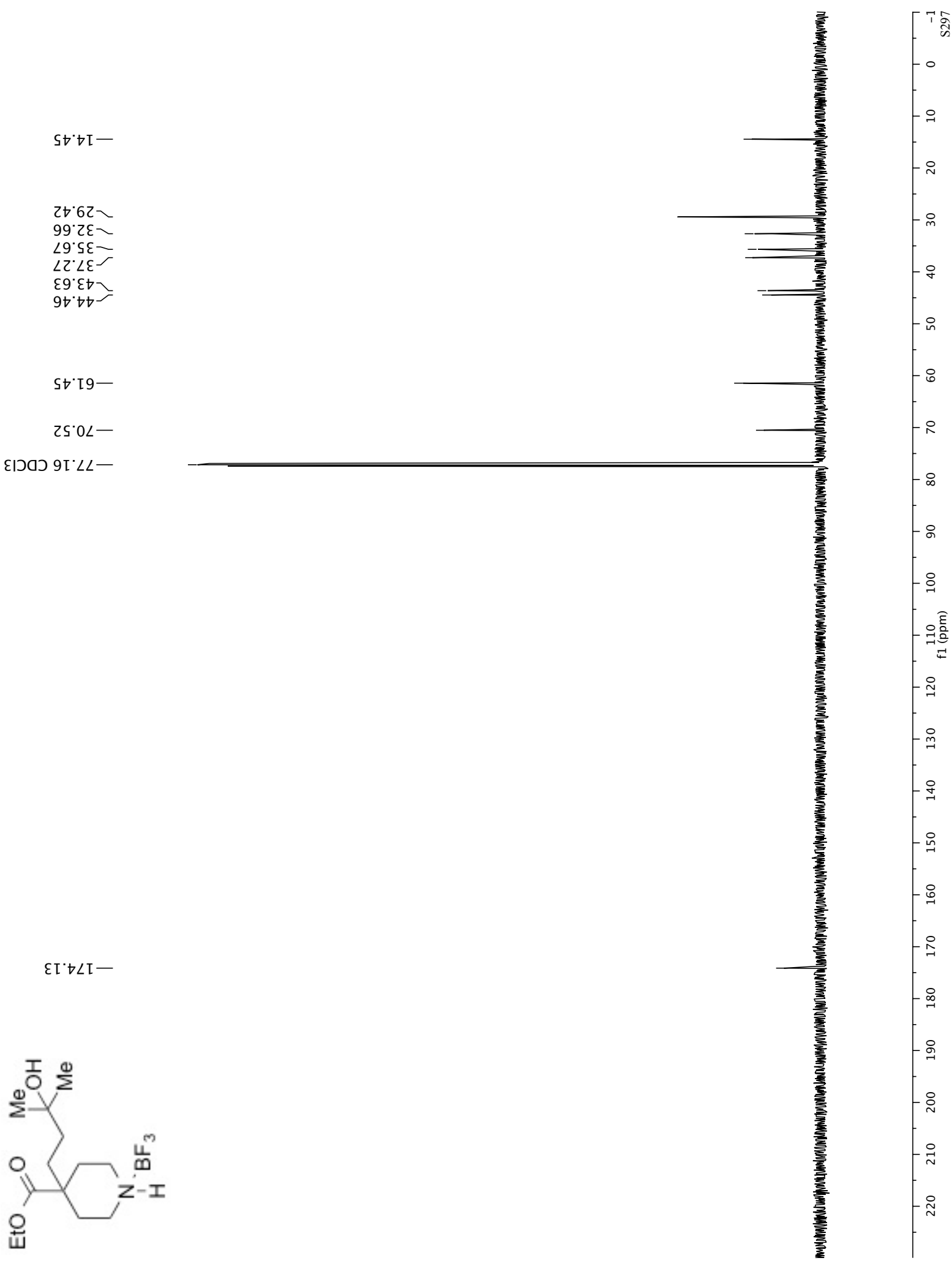
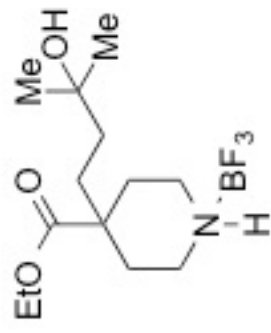
-158.11
-158.14
-158.18
-158.21

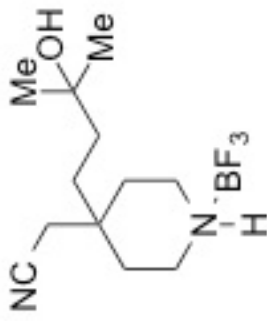




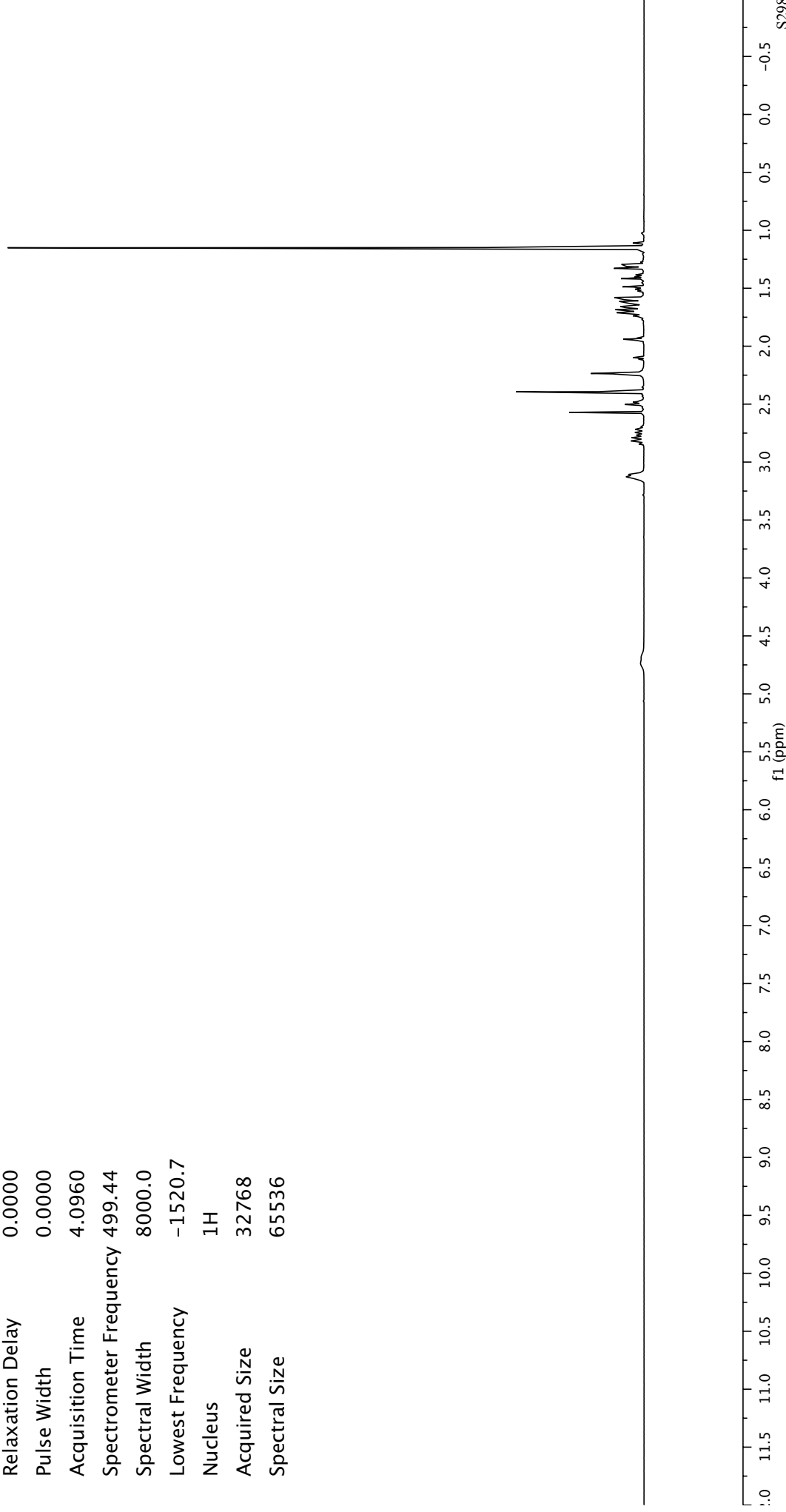
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	22.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	989
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1272.4
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

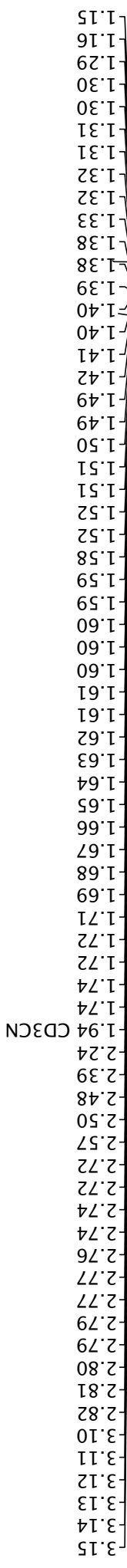
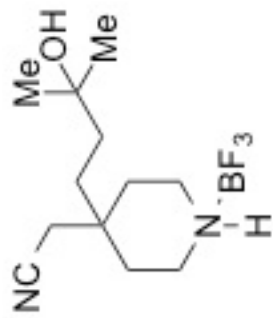
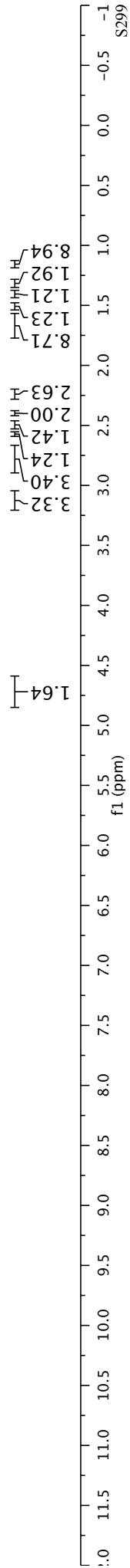


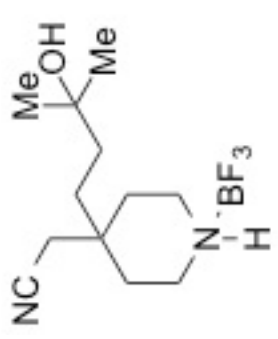
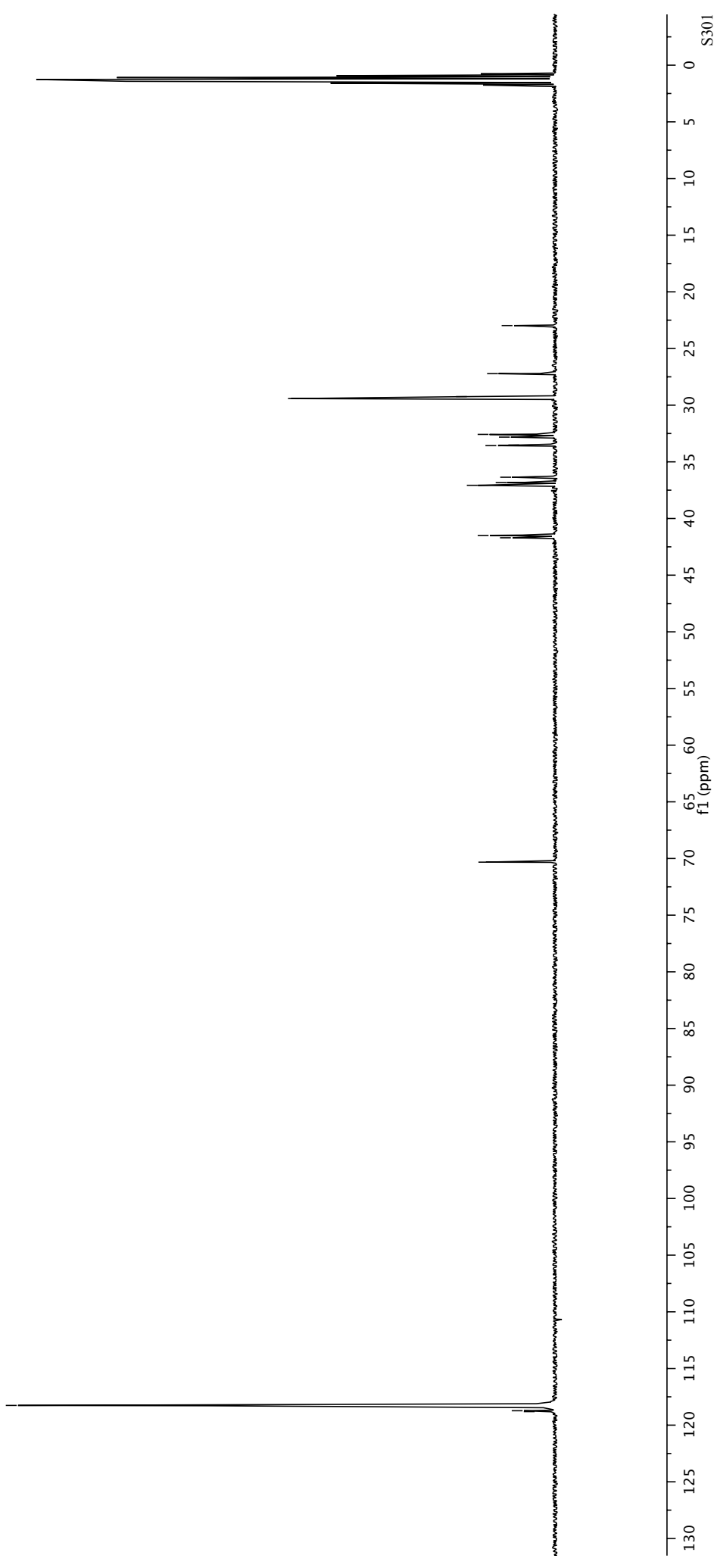




Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CD3CN
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Number of Scans	8
Receiver Gain	44
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	499.44
Spectral Width	8000.0
Lowest Frequency	-1520.7
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536



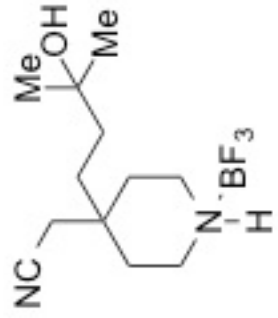




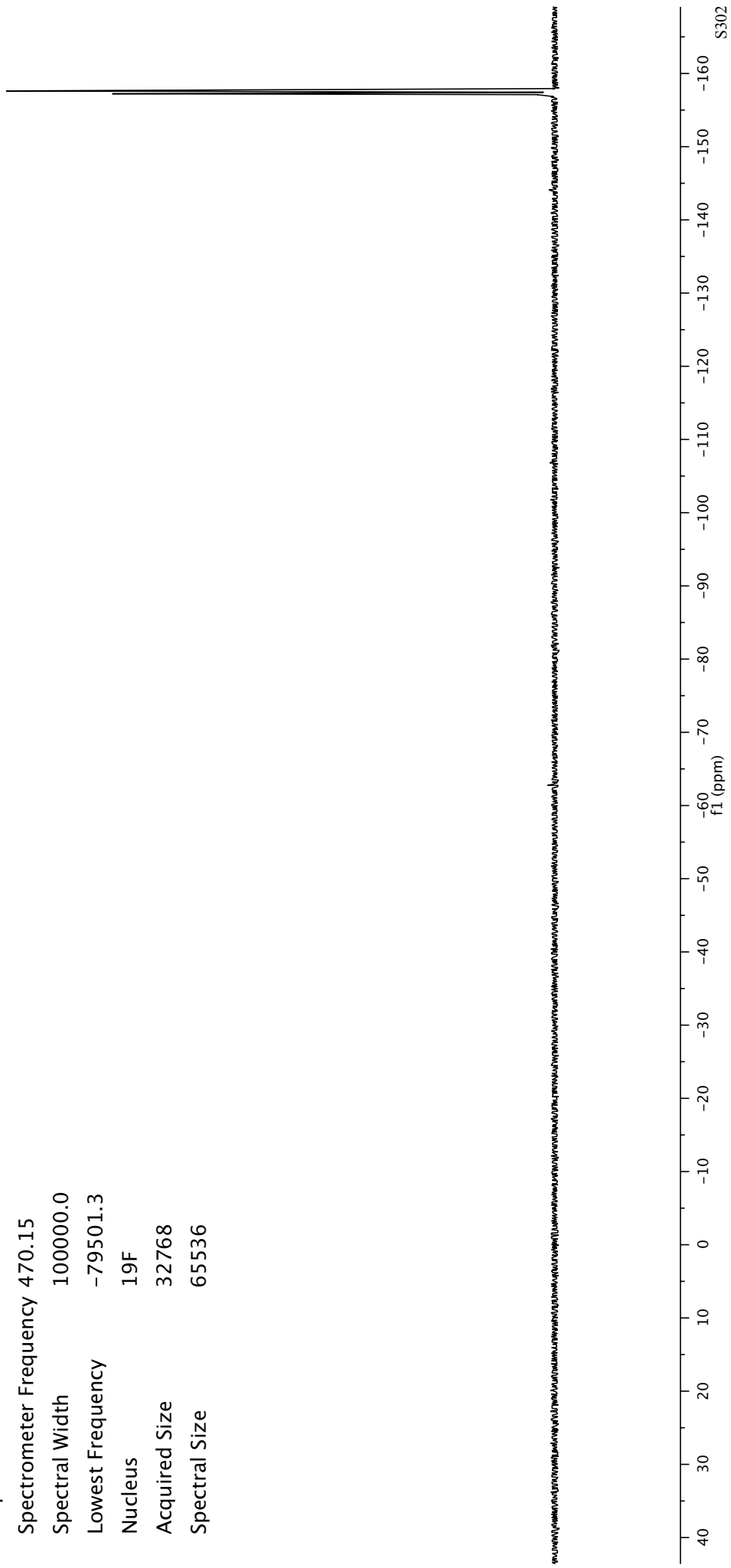
41.70
41.49
37.07
36.83
36.36
33.57
33.51
32.82
32.58
29.42
29.25
27.22
22.97

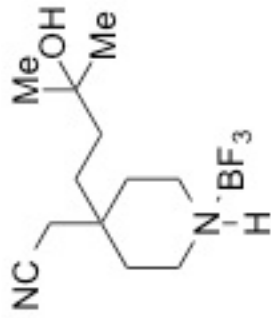
70.32
70.30

118.81
118.73
118.26 CD3CN



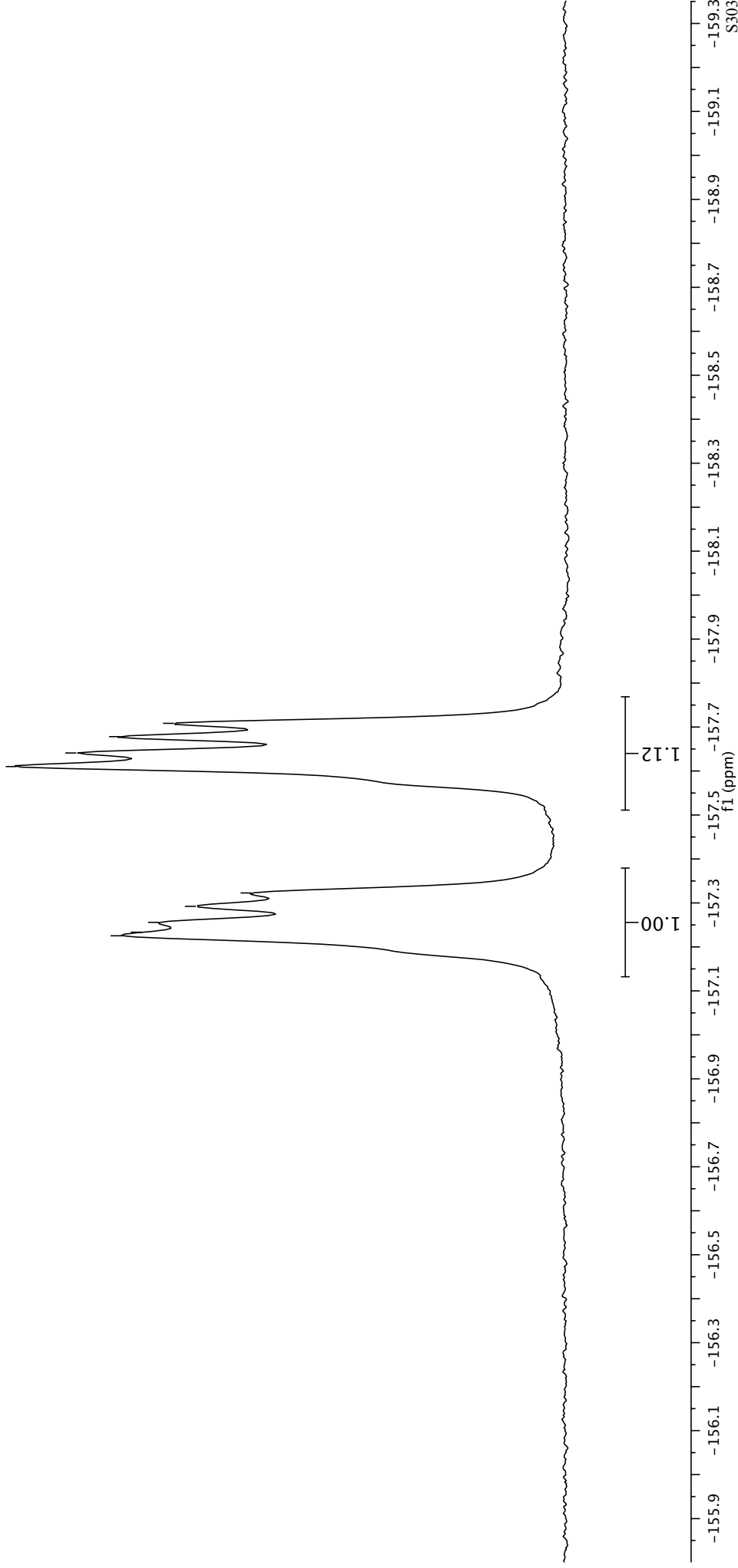
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	64
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency	-79501.3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

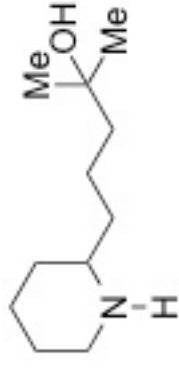




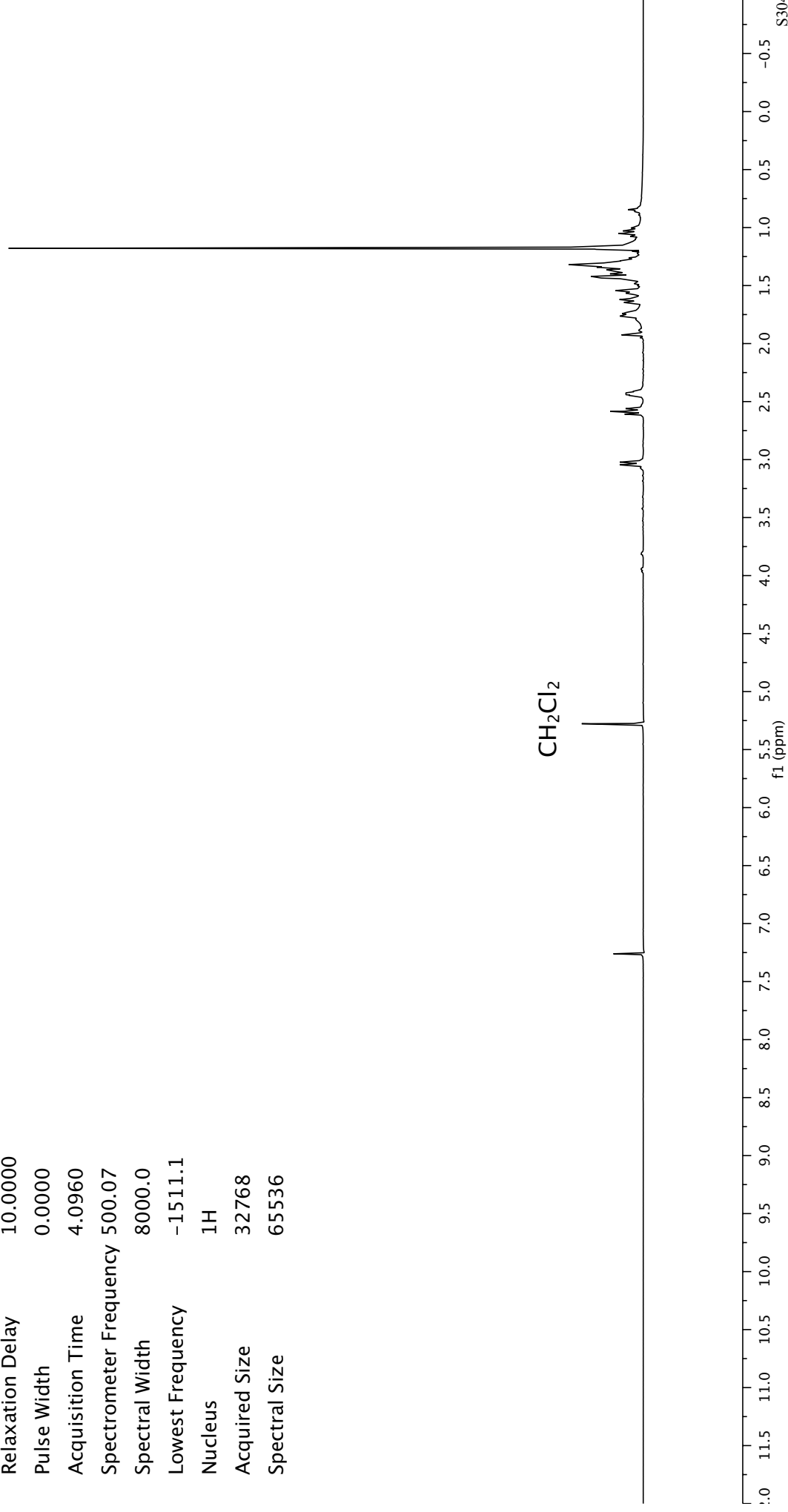
157.23
157.23
157.26
157.29
157.32

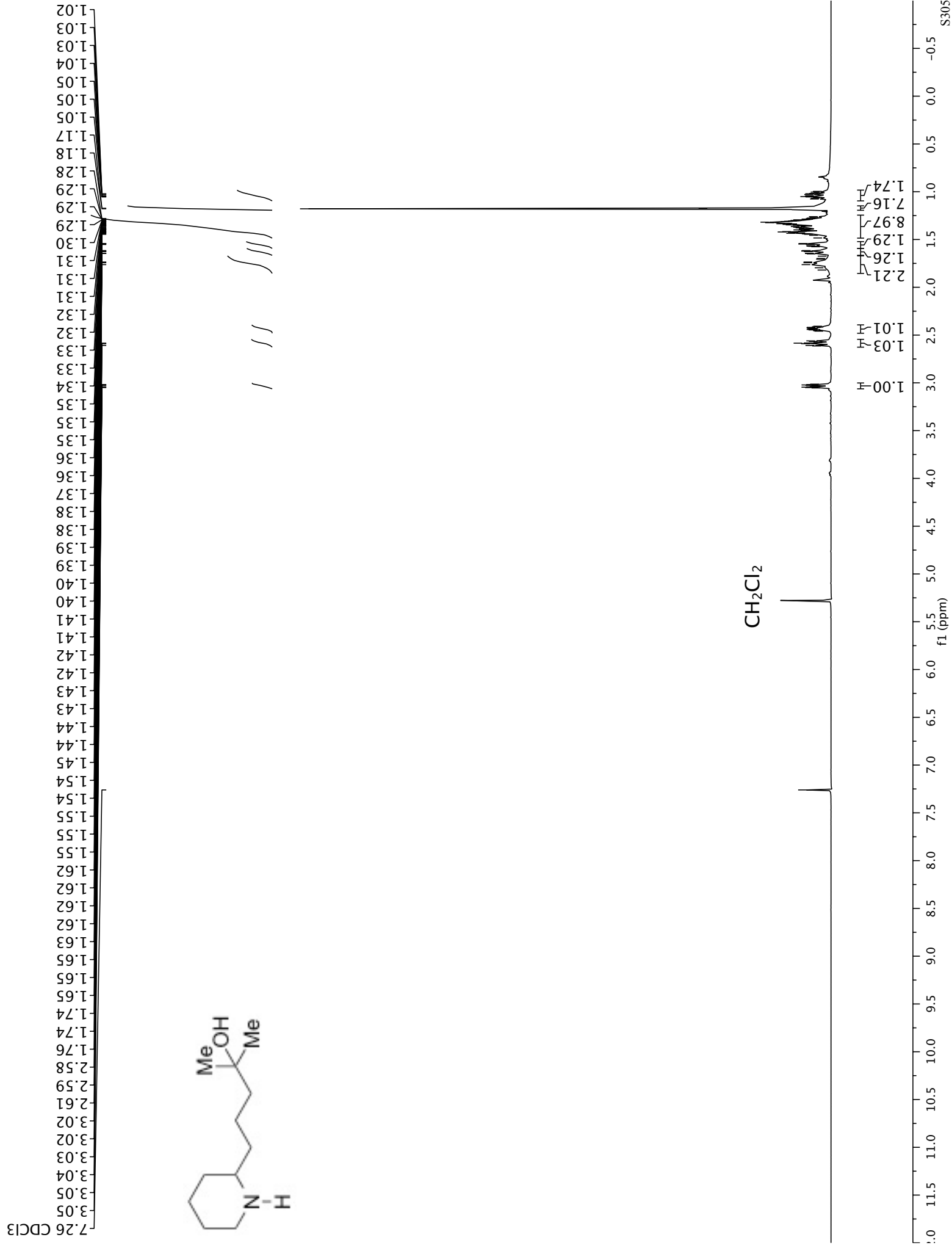
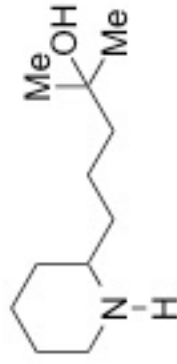
157.61
157.64
157.68
157.71

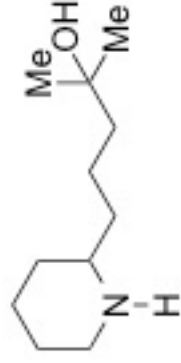




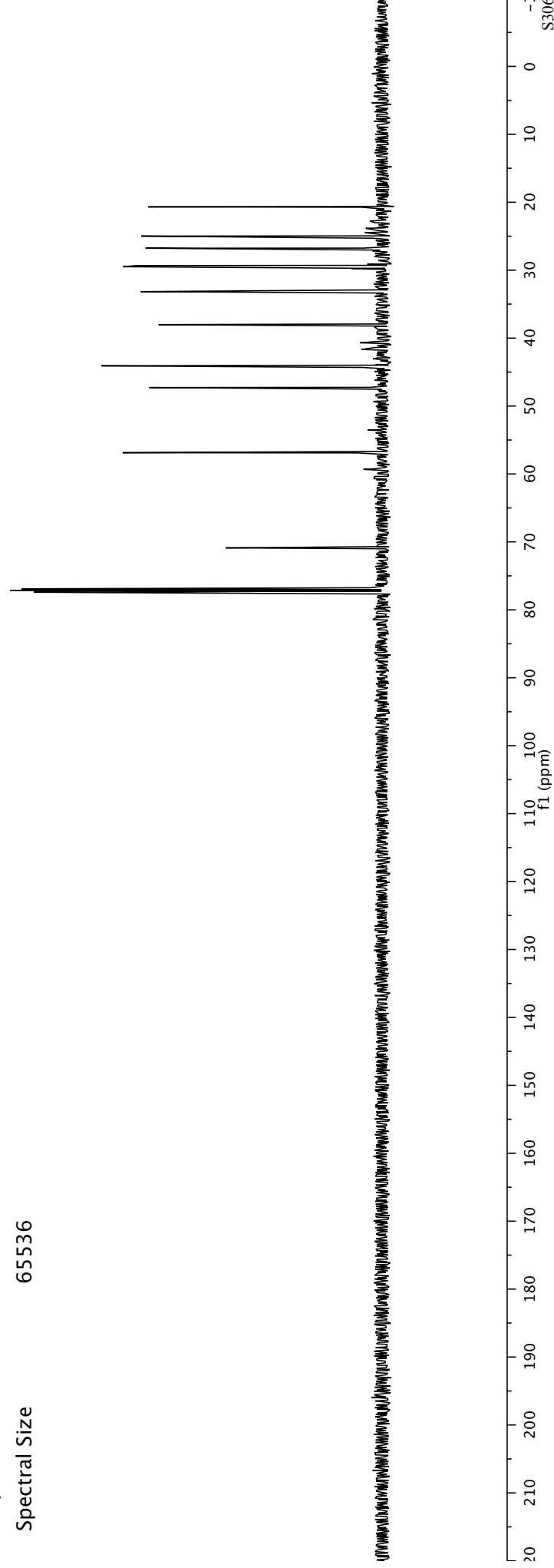
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	22
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1511.1
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

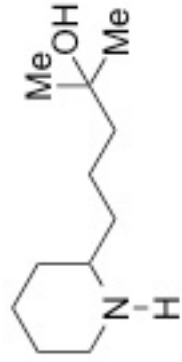




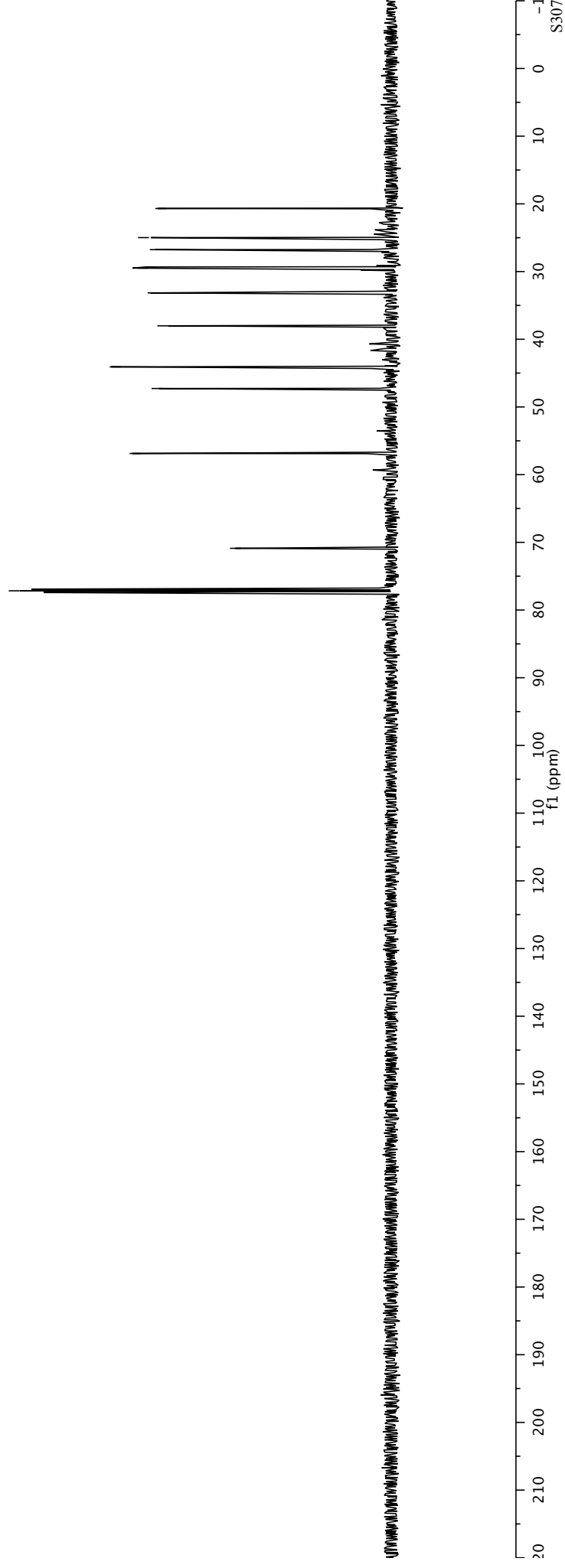


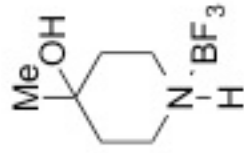
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	192
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1273.3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



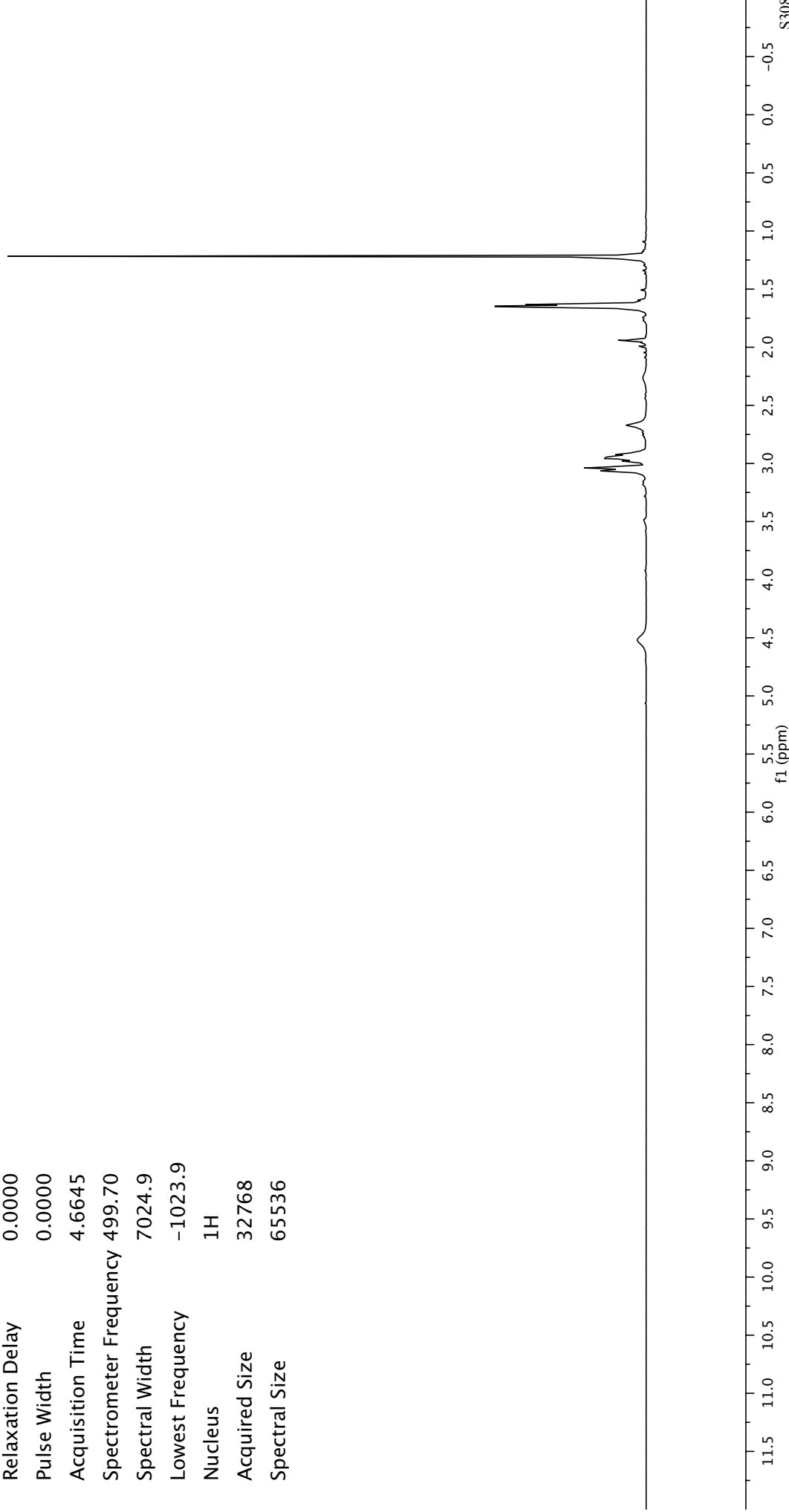


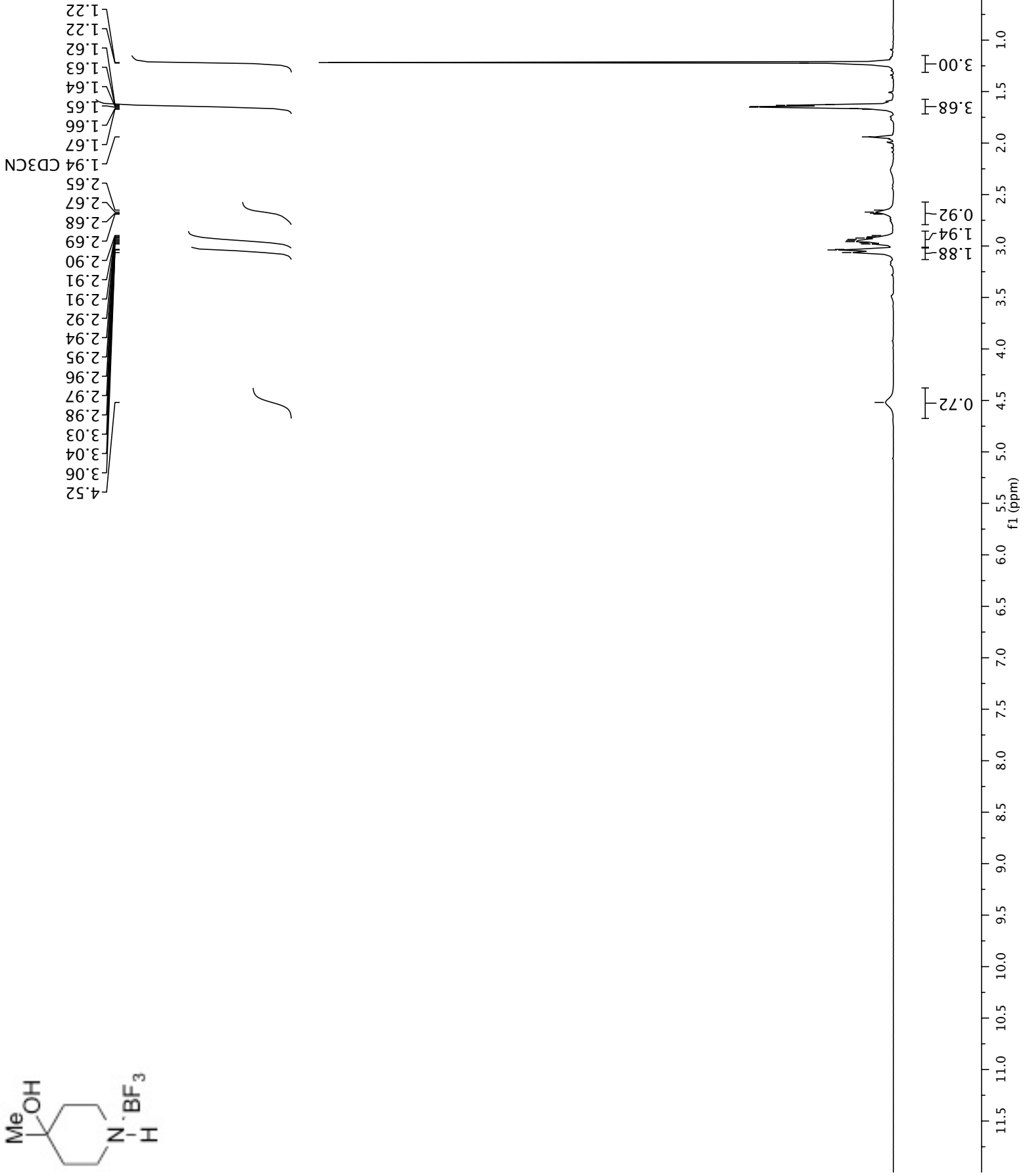
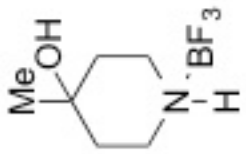
— 77.16 CDCl₃
 — 70.88
 — 56.87
 — 47.27
 — 44.08
 — 38.02
 — 33.15
 — 29.49
 — 29.32
 — 26.77
 — 24.98
 — 20.69

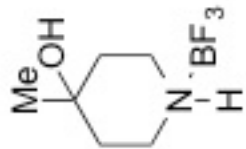




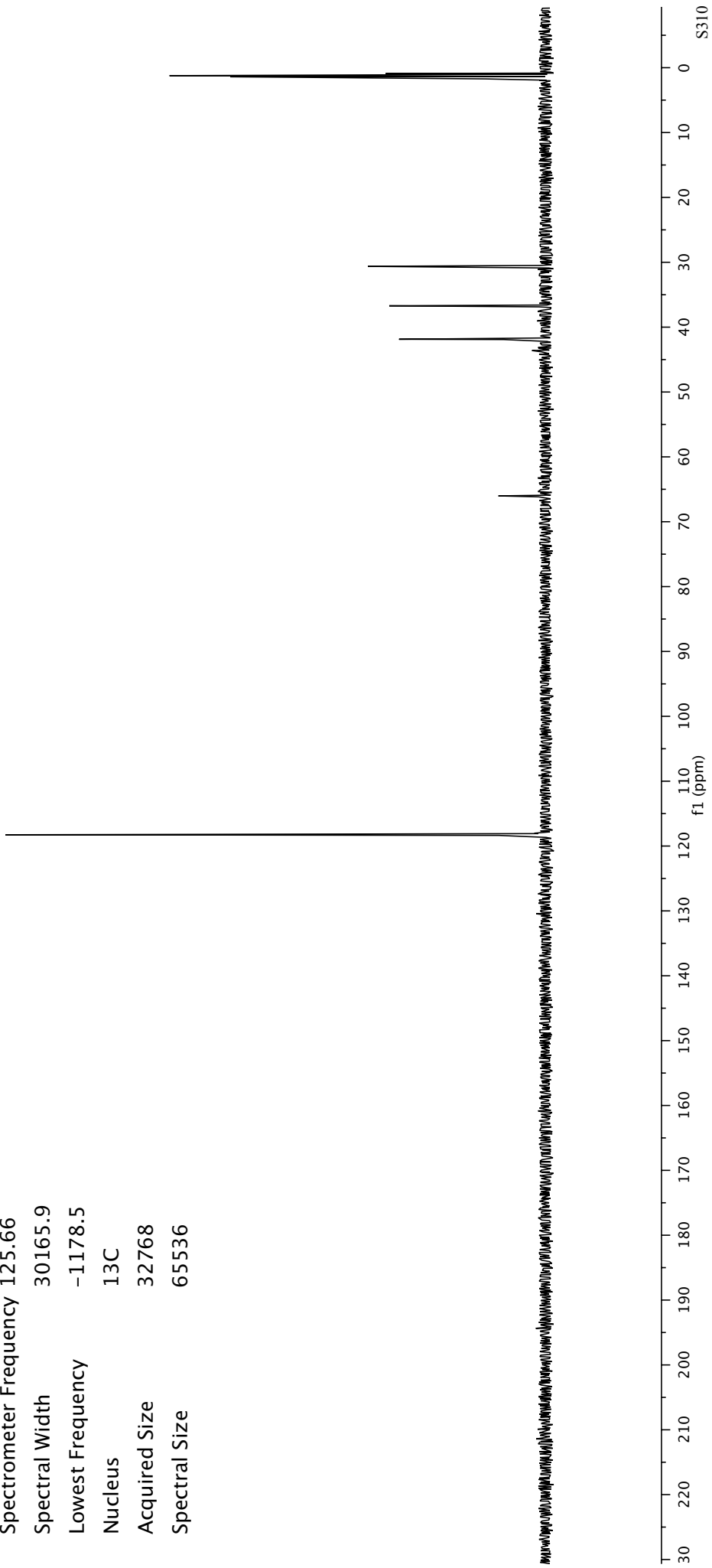
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CD3CN
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	8
Receiver Gain	41
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.70
Spectral Width	7024.9
Lowest Frequency	-1023.9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

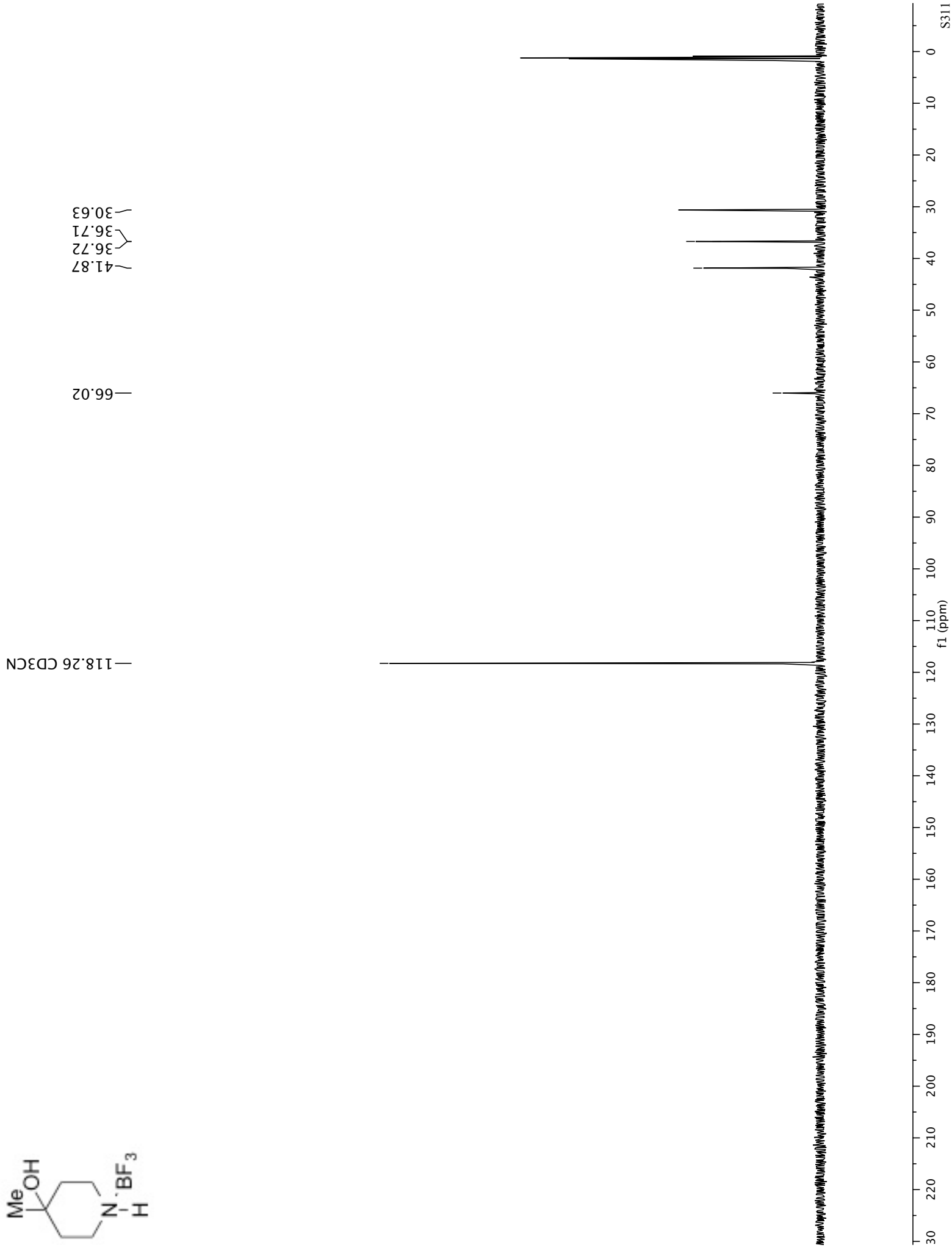
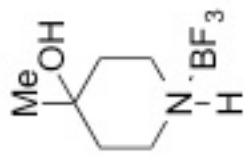


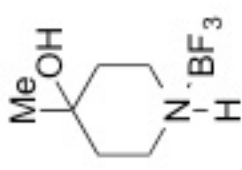




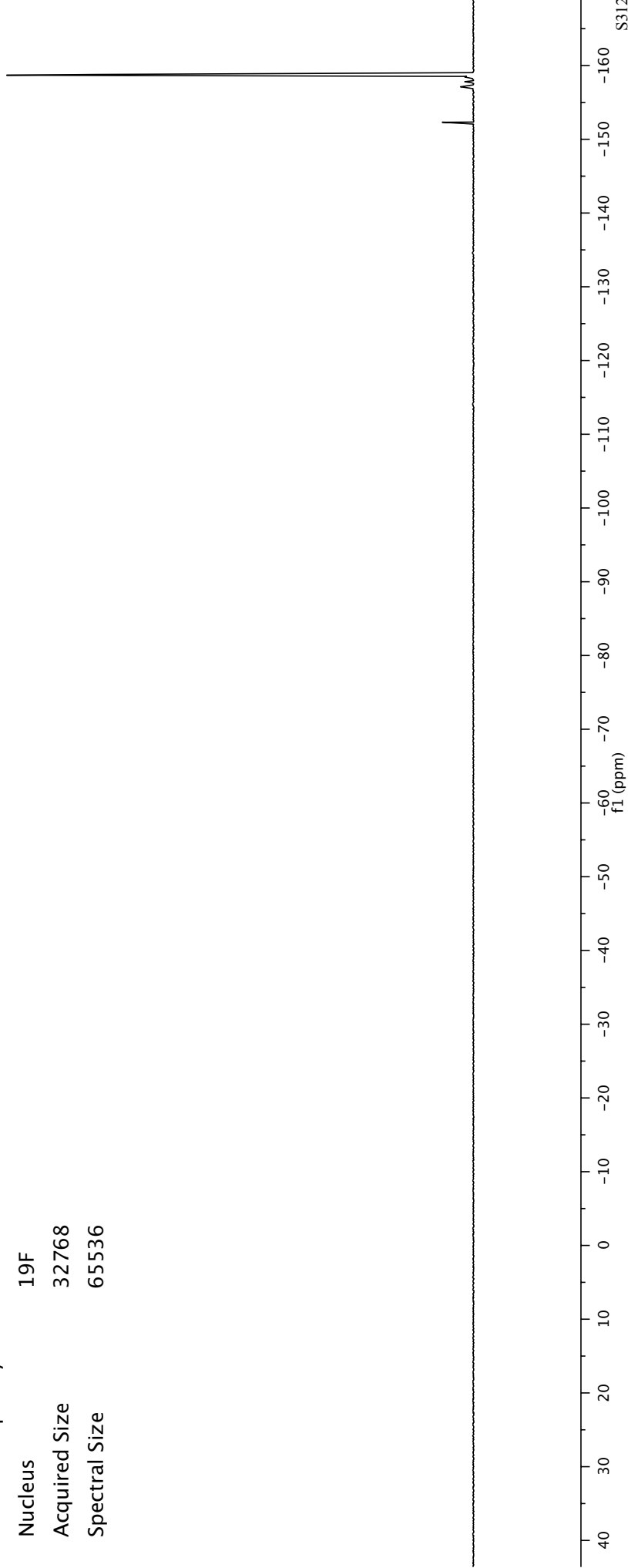
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CD3CN
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	112
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1178.5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

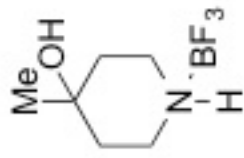




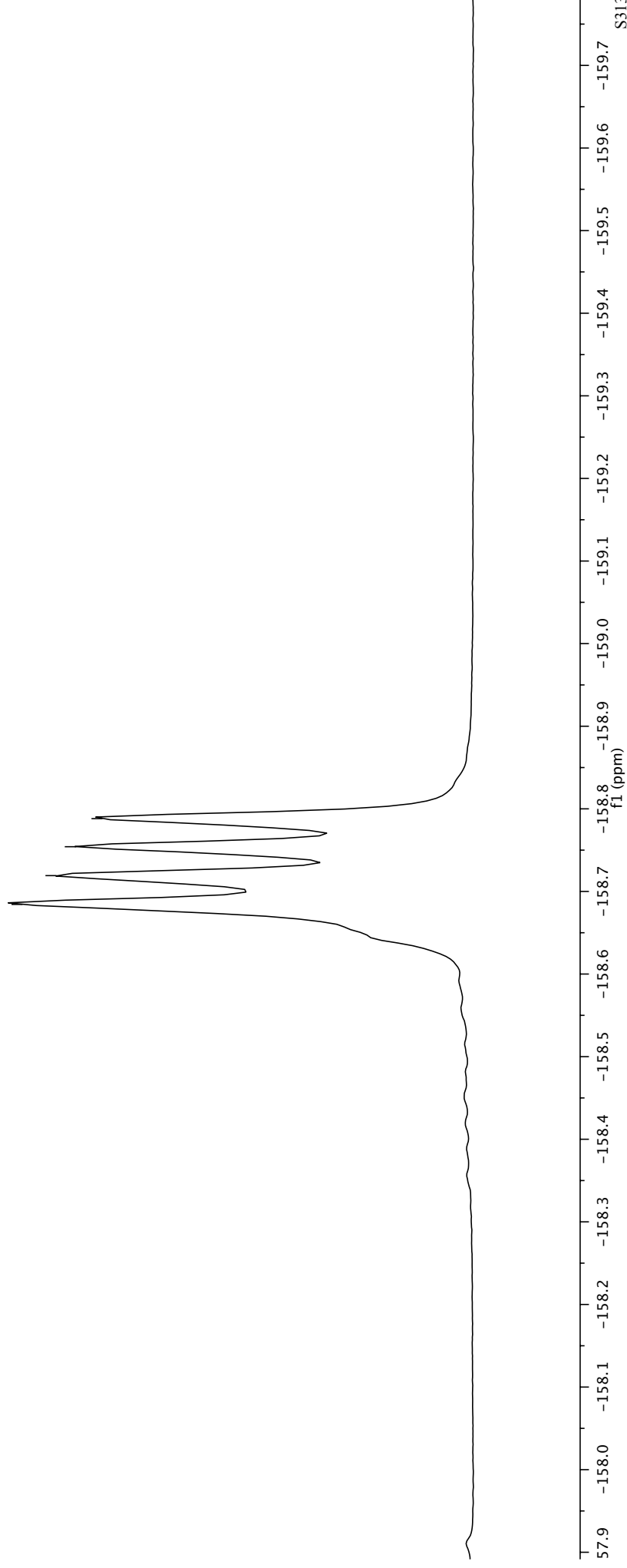


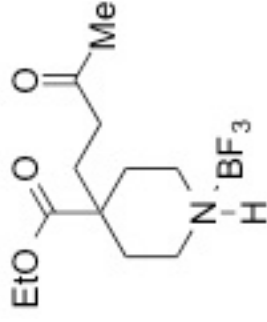
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CD3CN
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	128
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency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



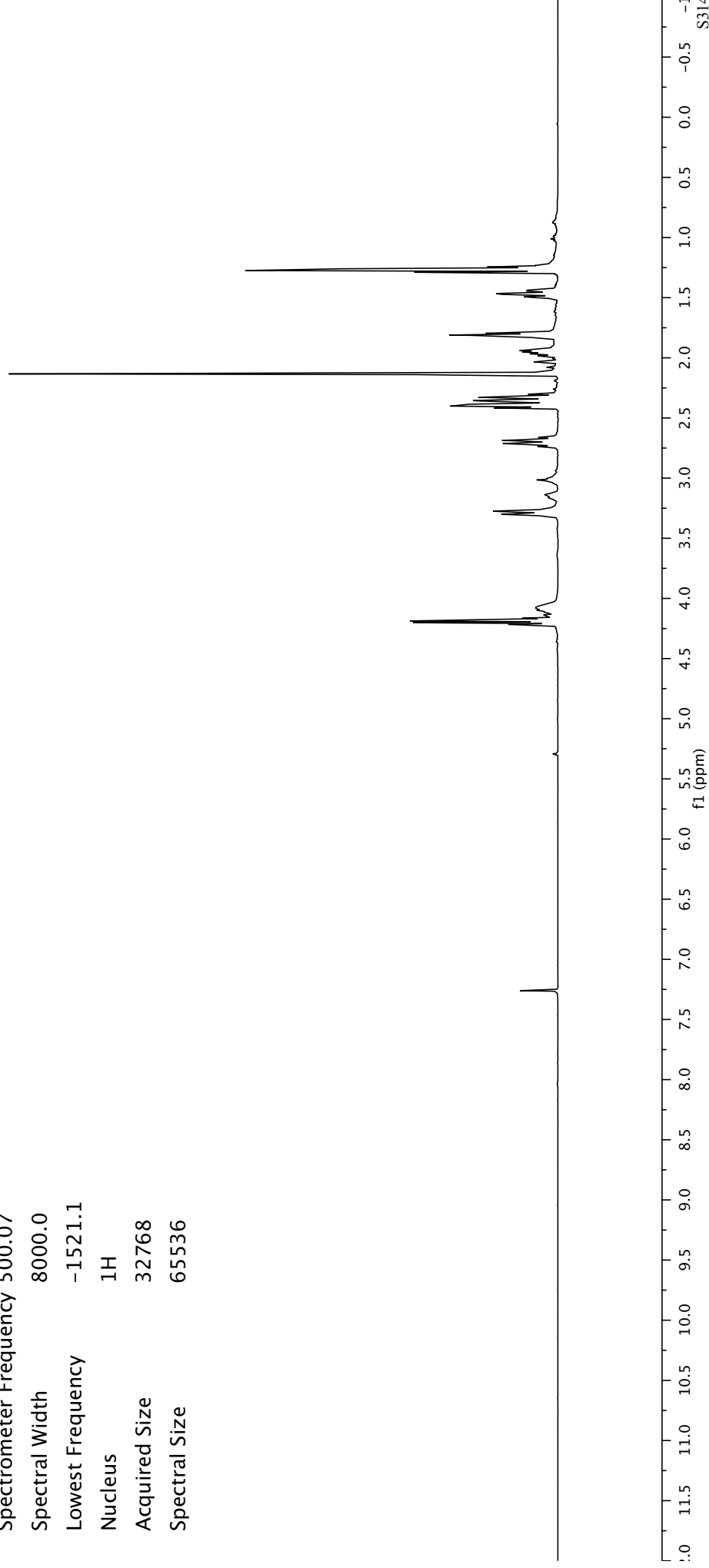


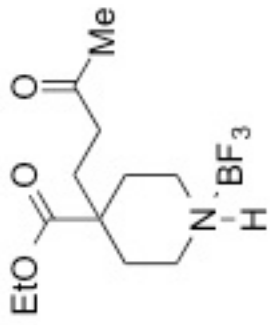
~158.68
~158.72
~158.75
~158.79



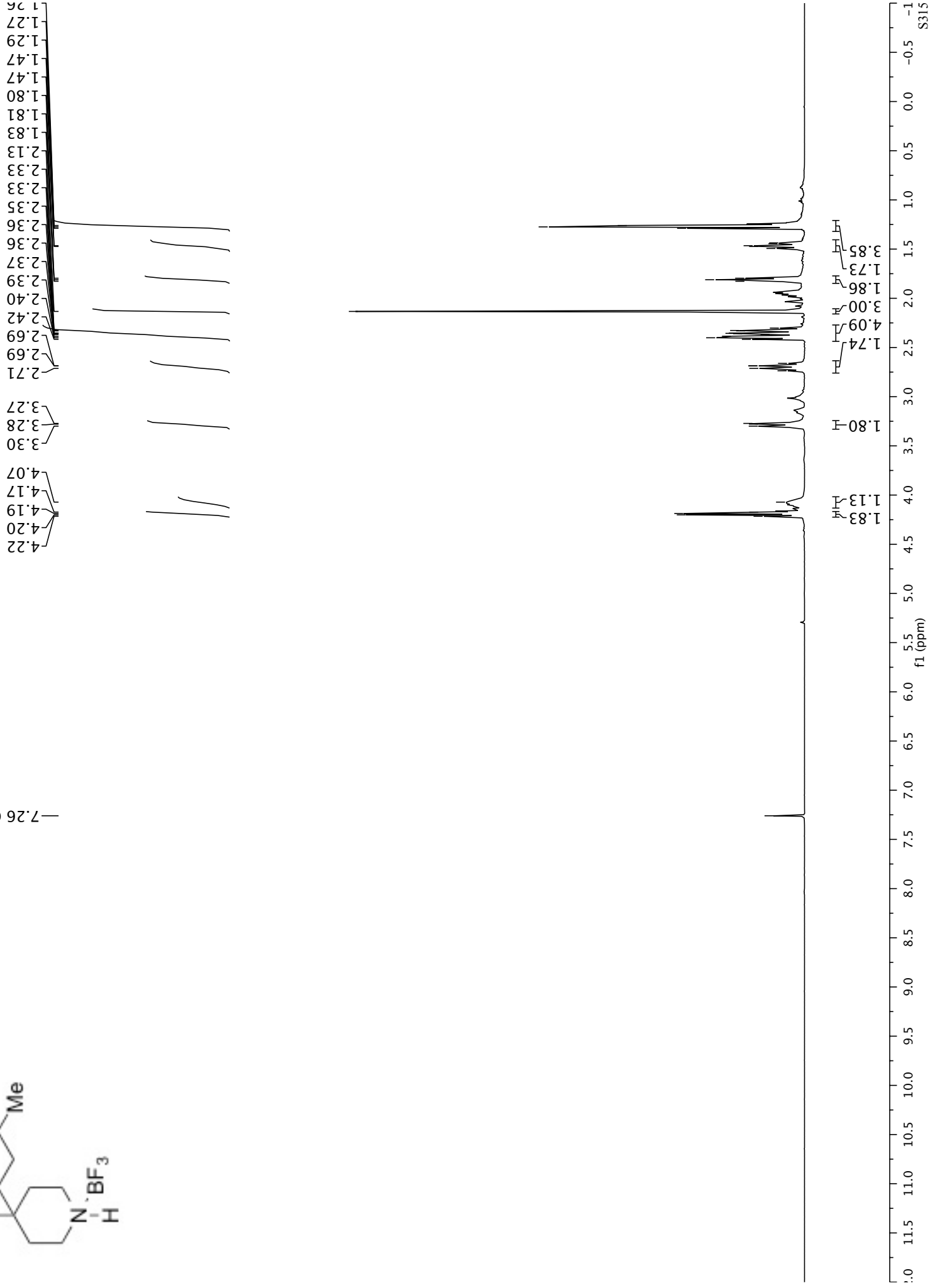


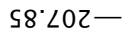
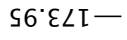
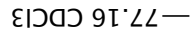
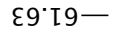
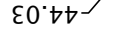
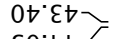
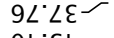
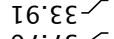
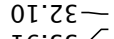
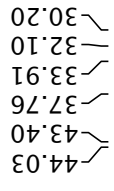
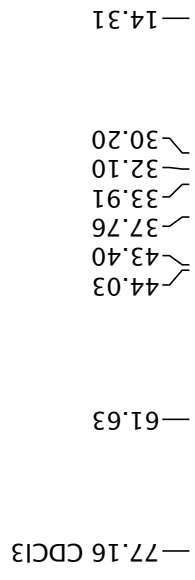
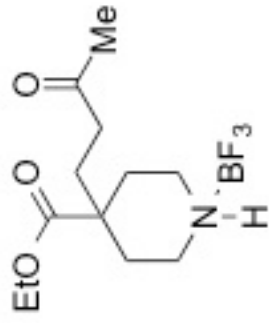
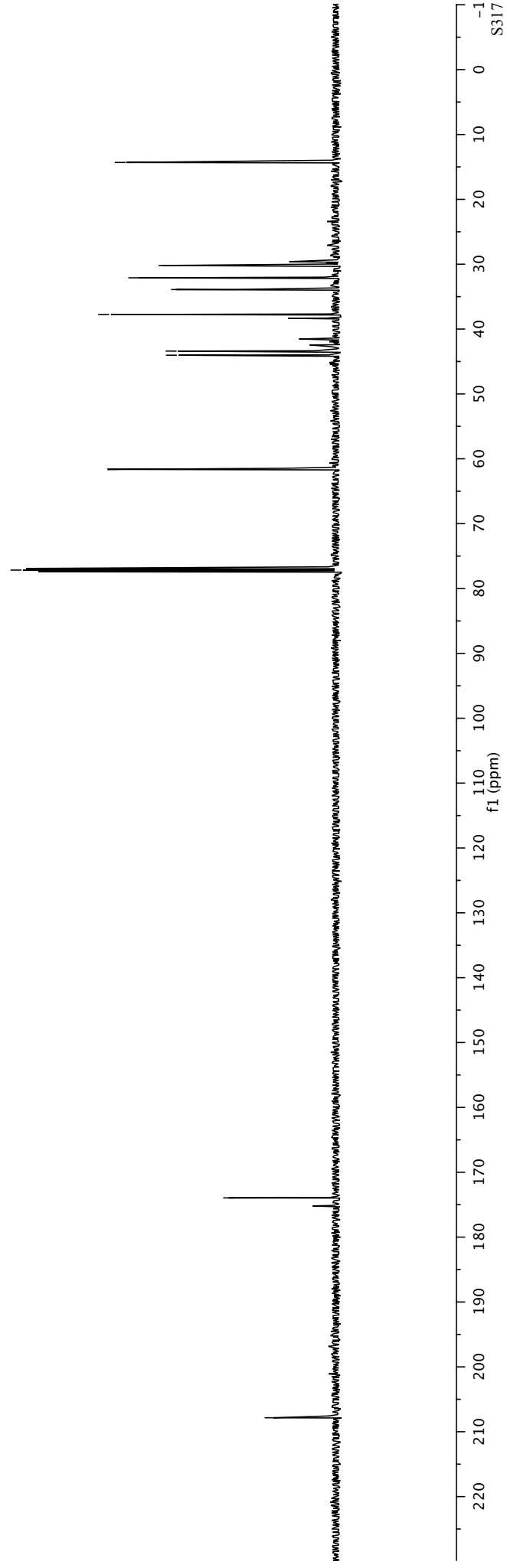
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	26
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

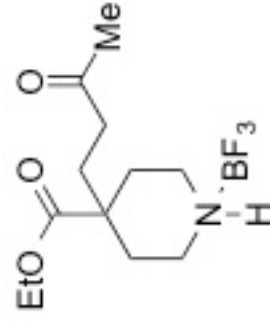




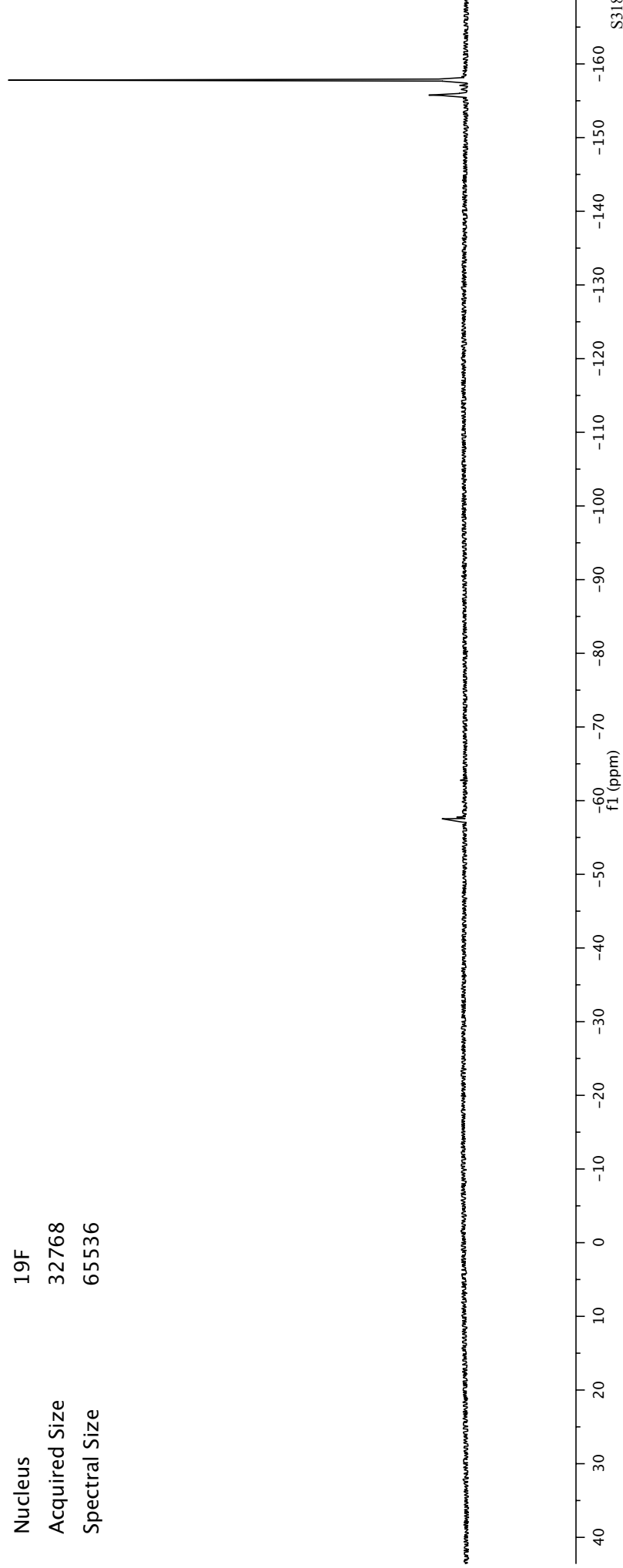
—7.26 CDCl₃

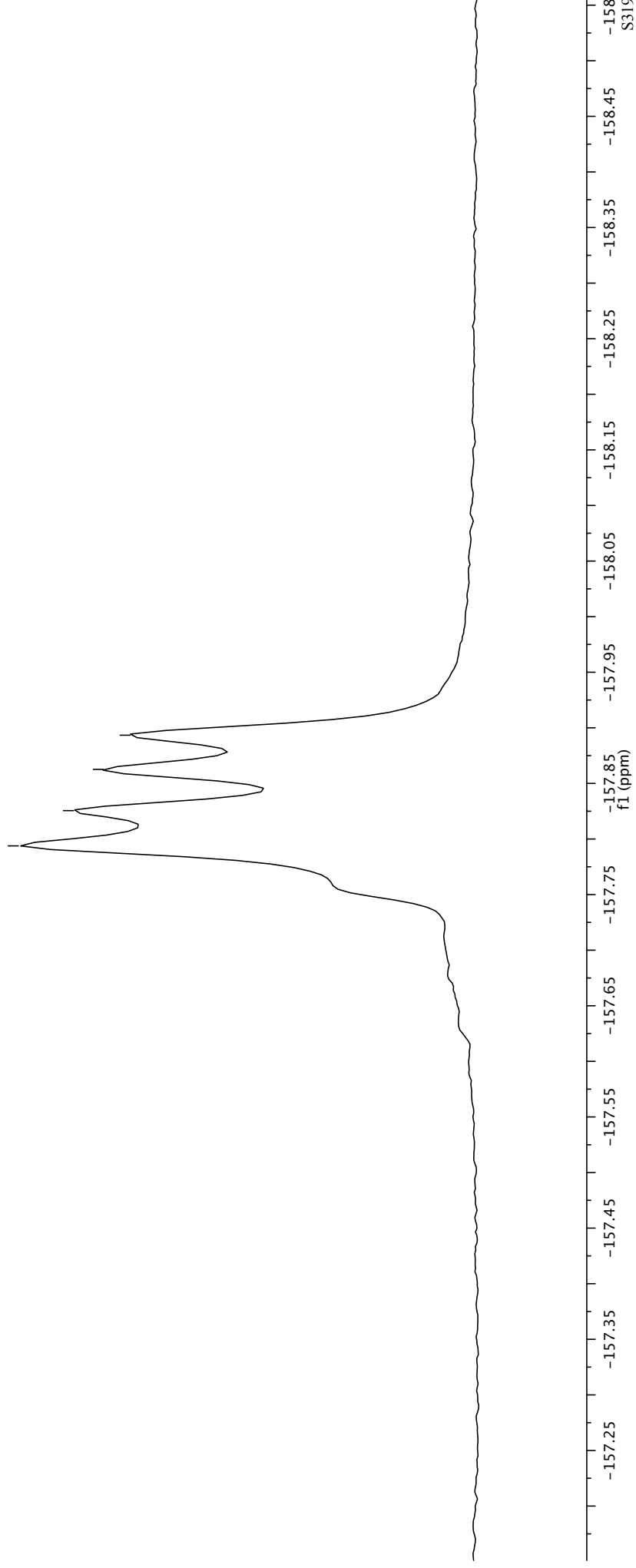
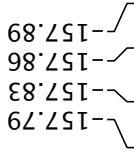
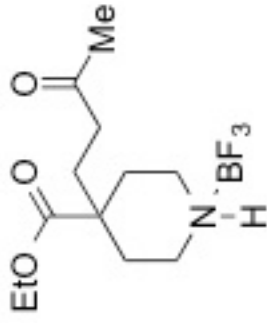


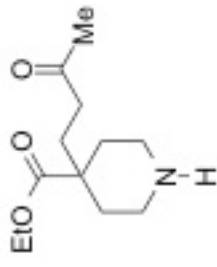




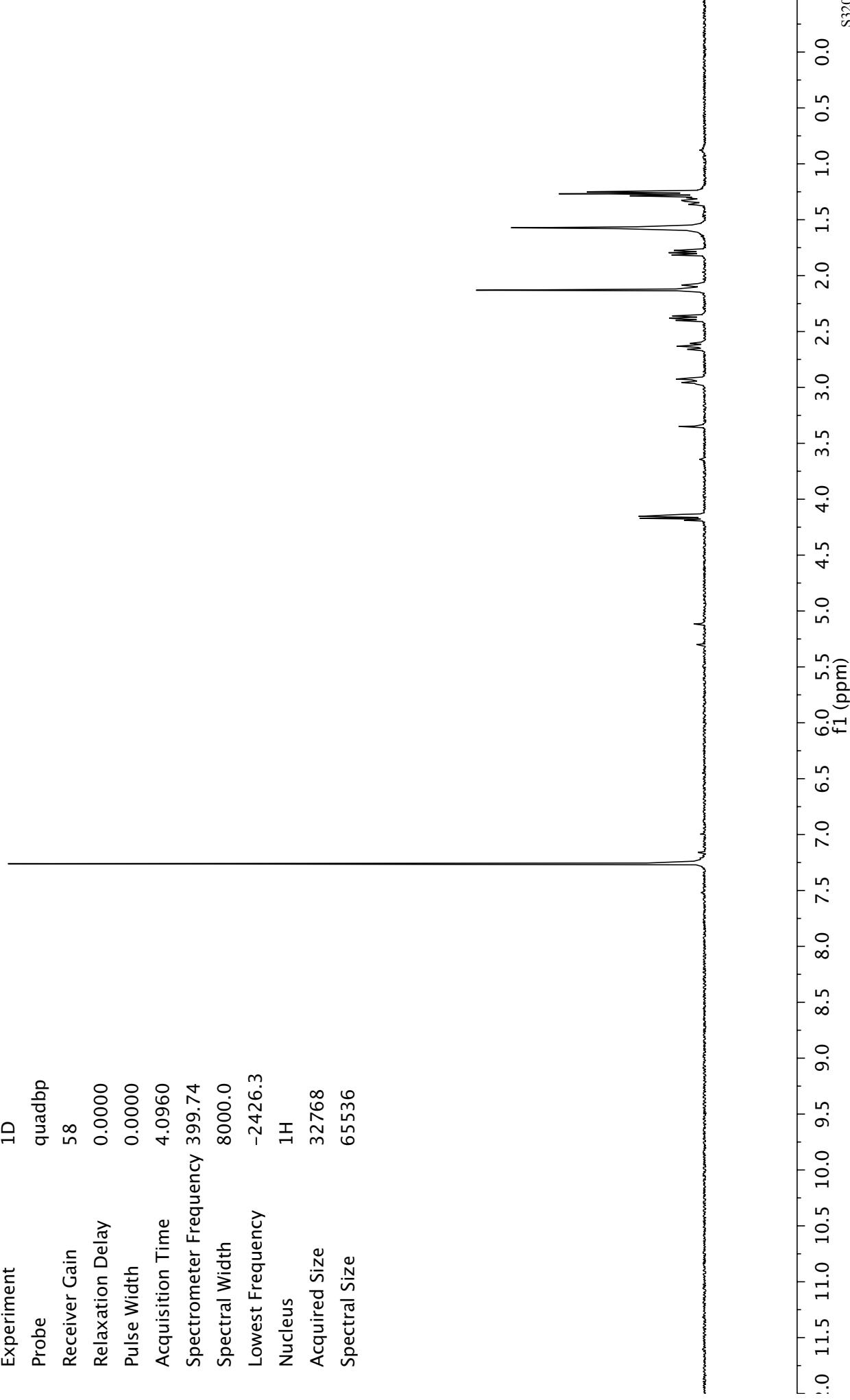
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	132
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency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

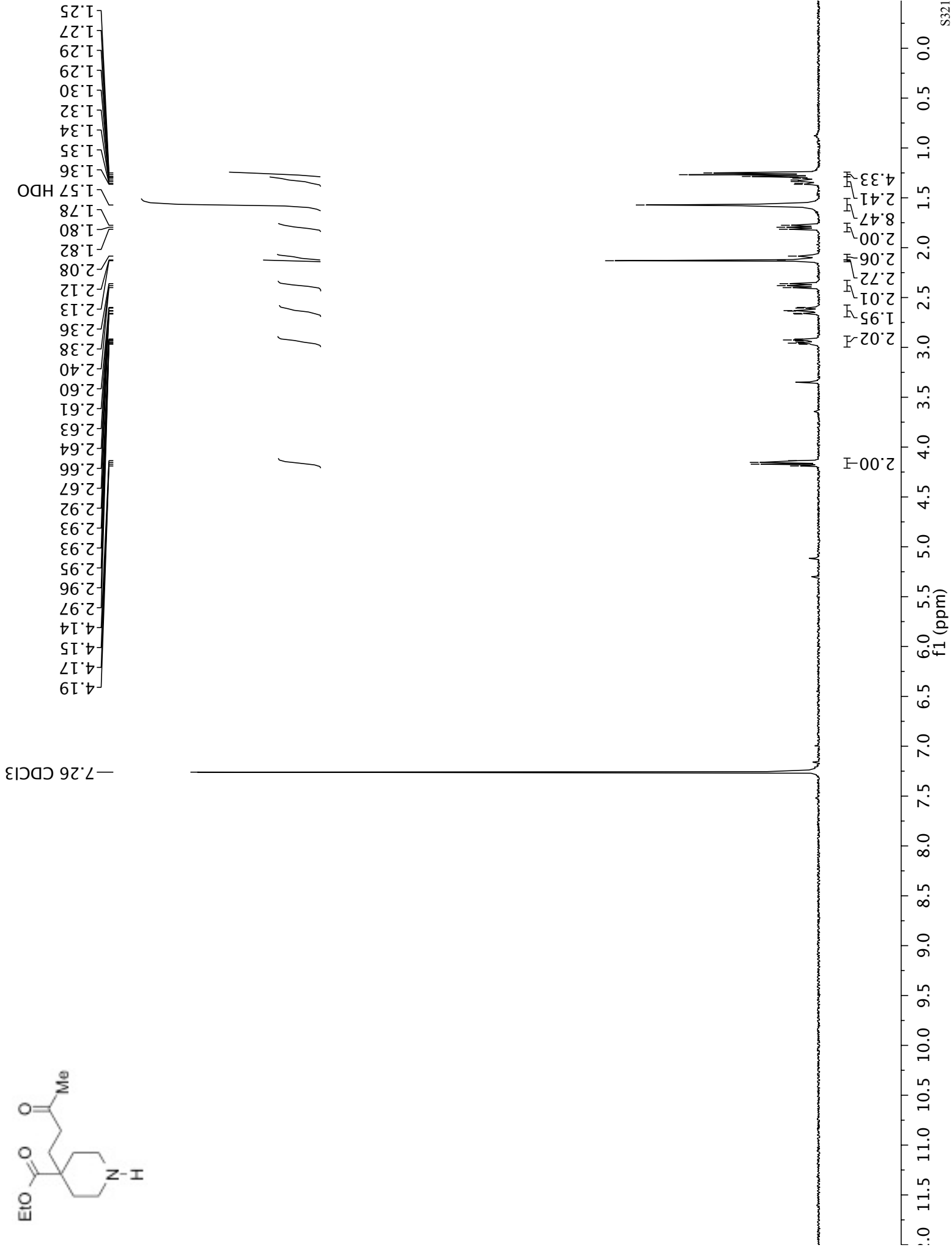
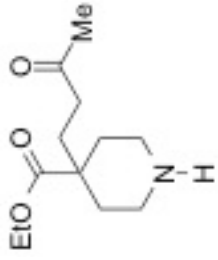




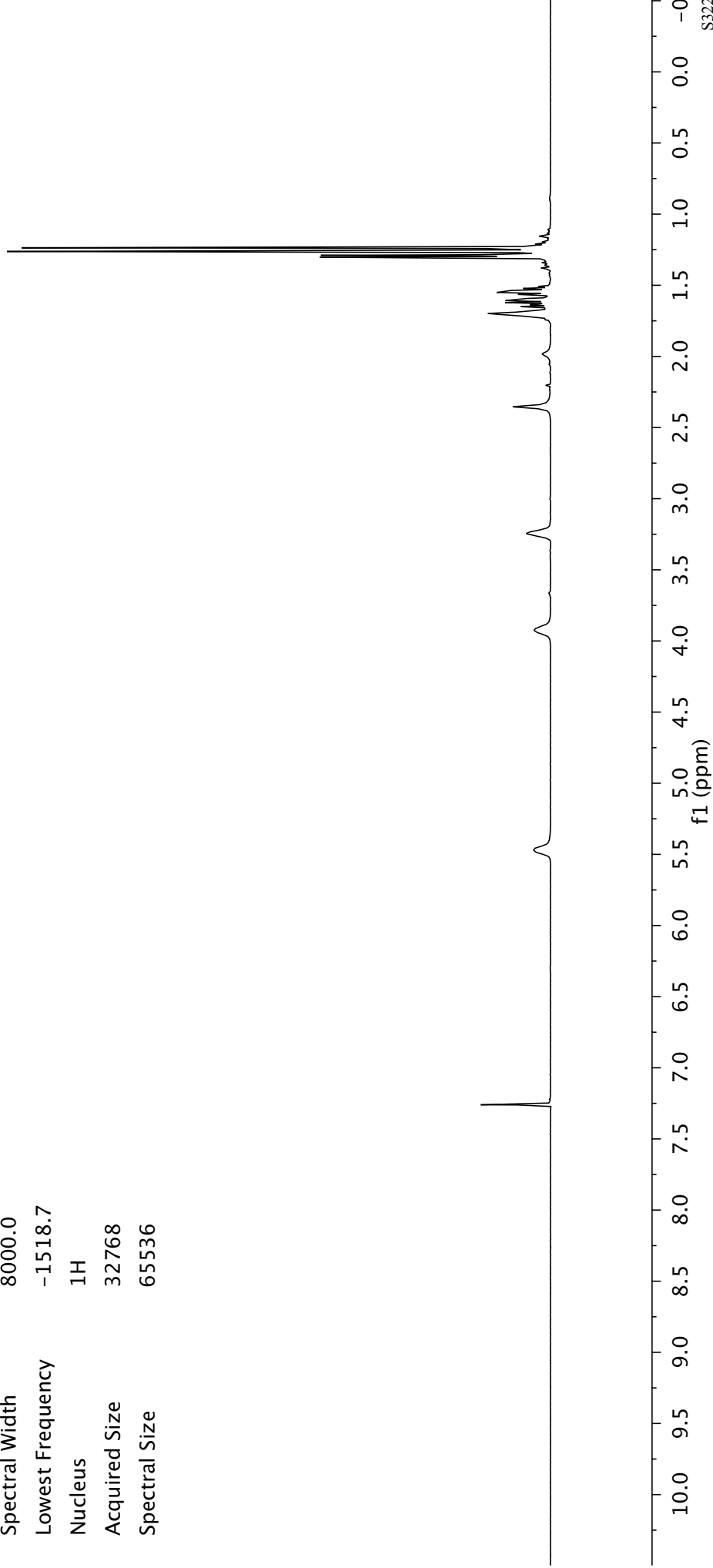
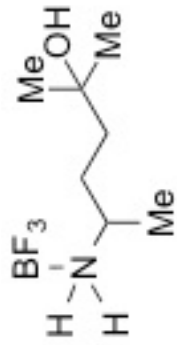


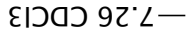
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quadbp
Receiver Gain	58
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	399.74
Spectral Width	8000.0
Lowest Frequency	-2426.3
Nucleus	¹ H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



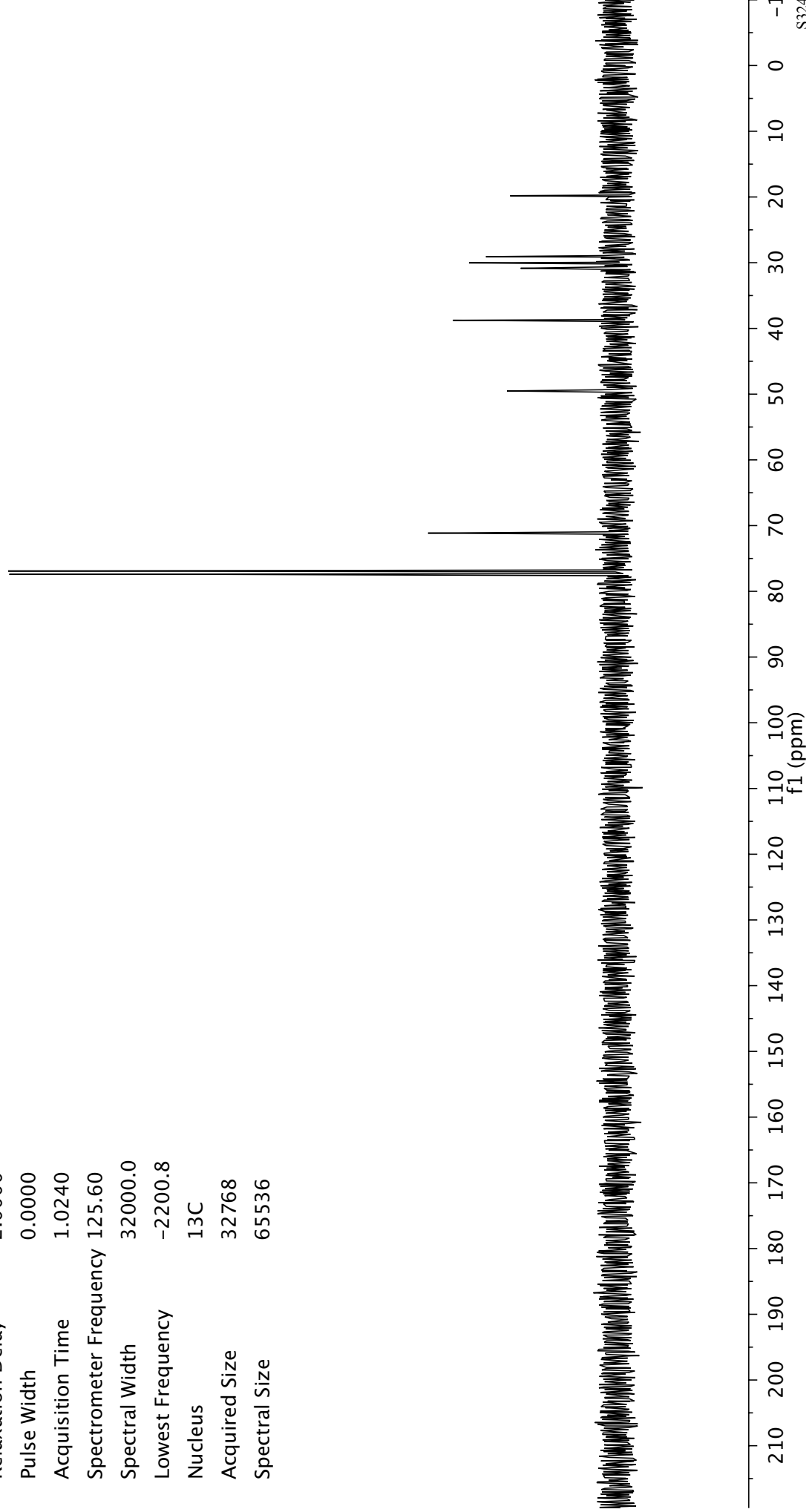
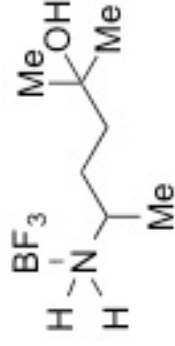


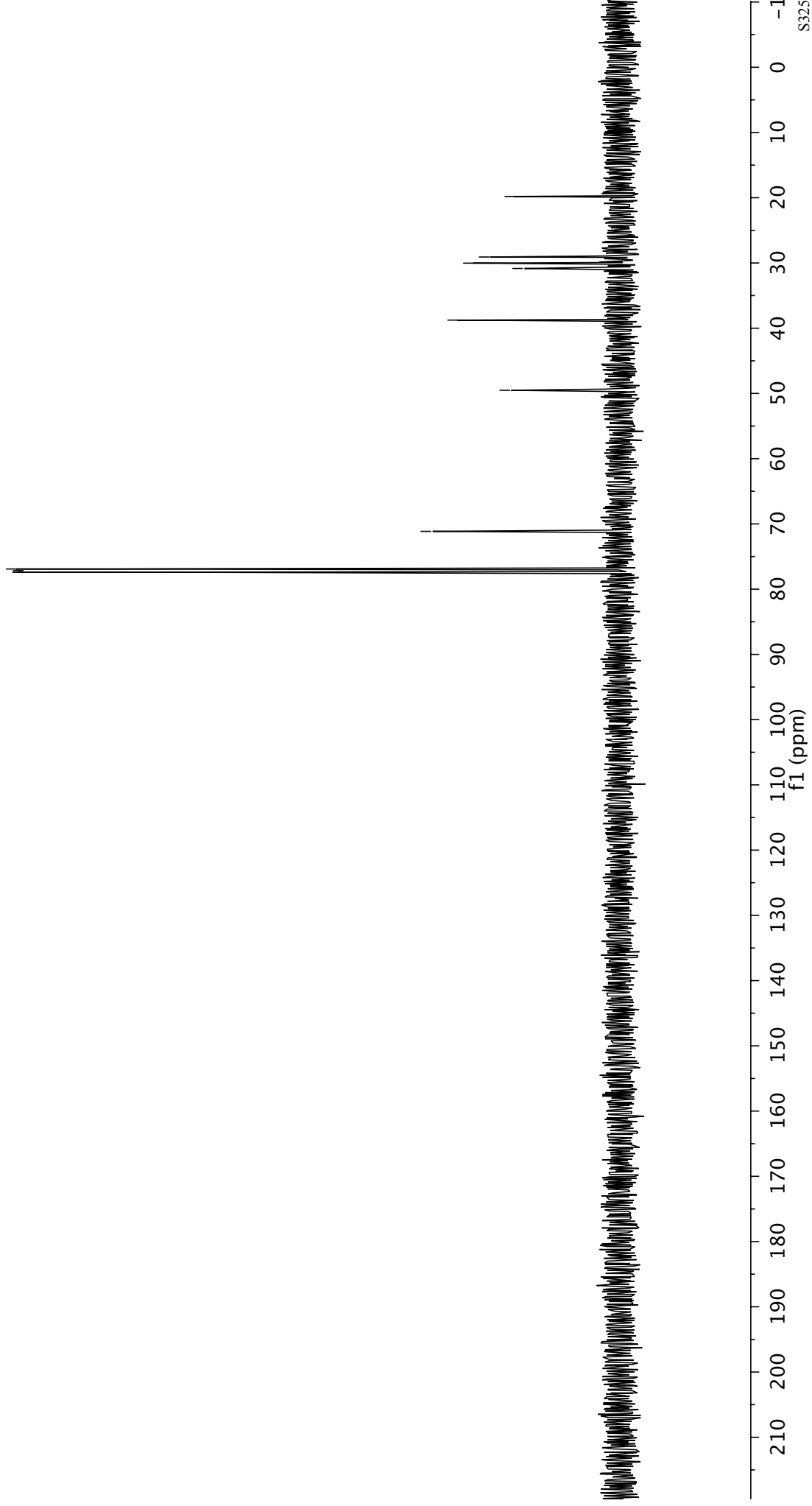
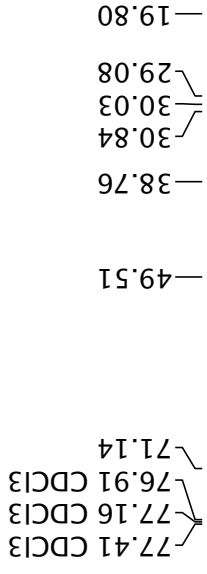
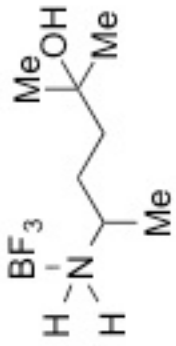
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	56
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	499.43
Spectral Width	8000.0
Lowest Frequency	-1518.7
Nucleus	1H
Acquired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

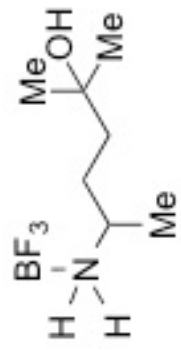




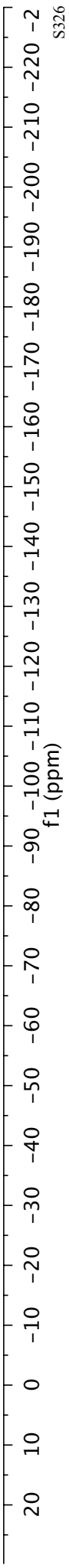
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2200.8
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

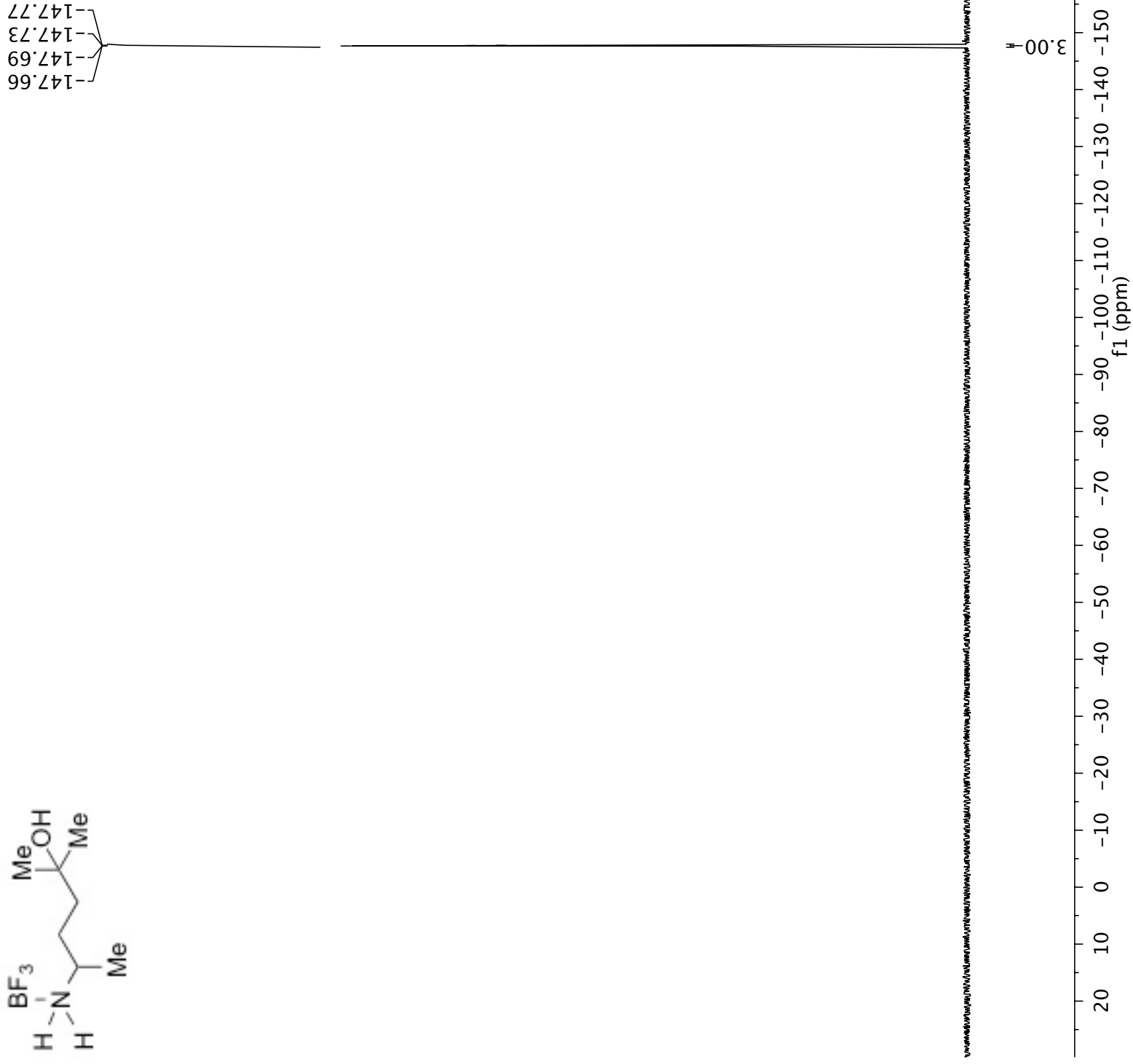
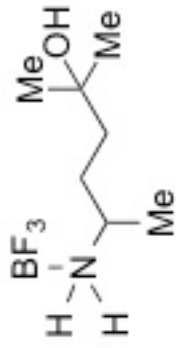


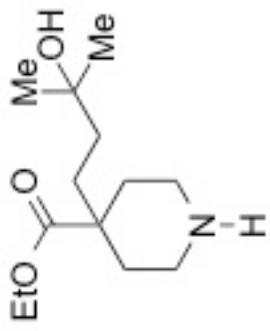




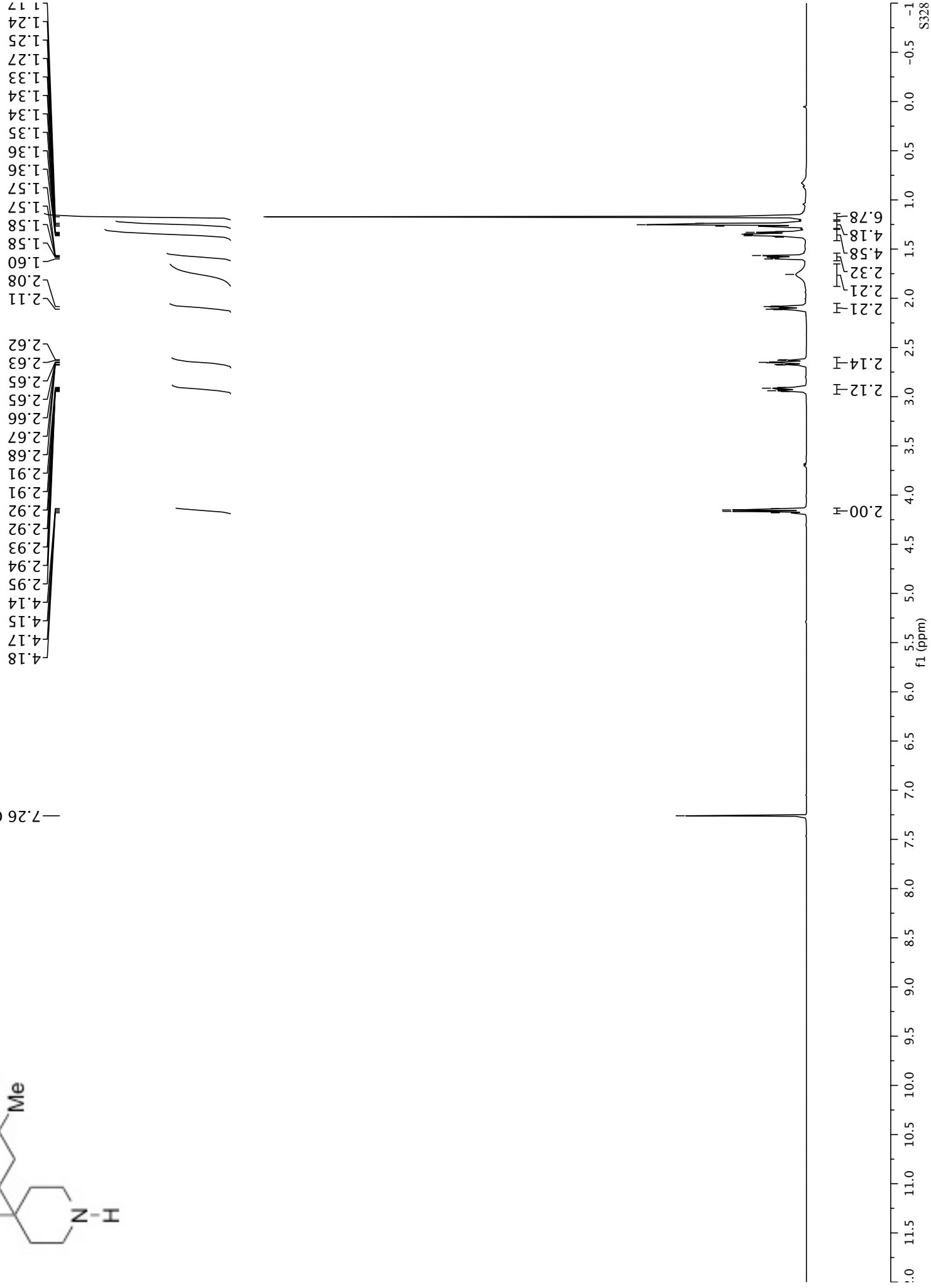
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	56
Relaxation Delay	1.5000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	469.89
Spectral Width	122137.4
Lowest Frequency	-108111.4
Nucleus	19F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

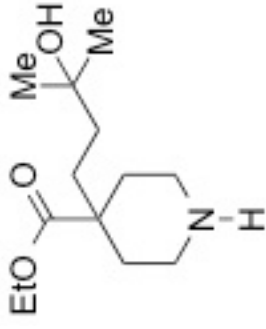




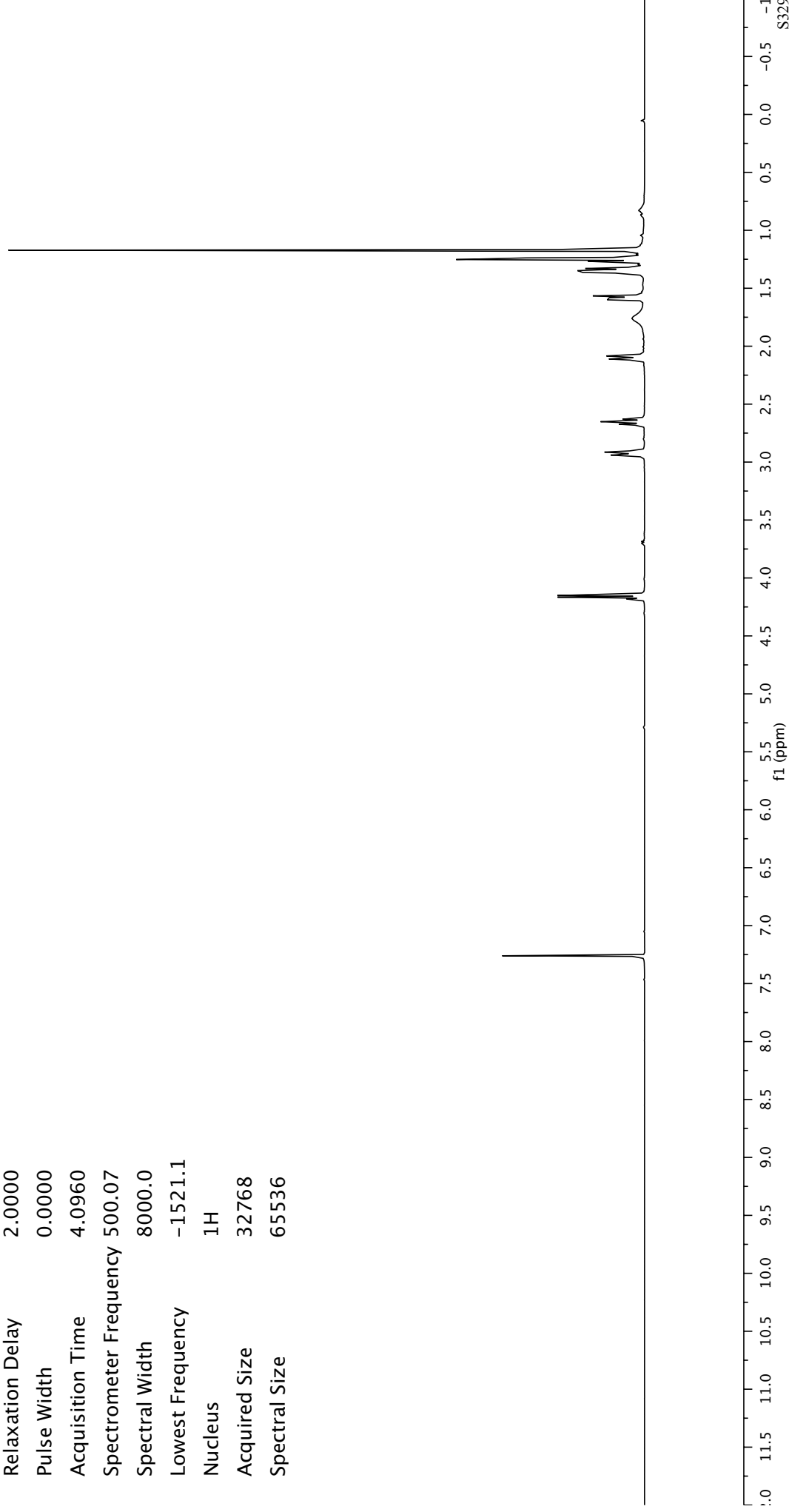


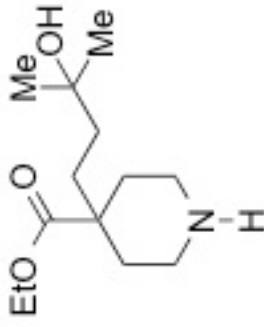
—7.26 CDCl₃



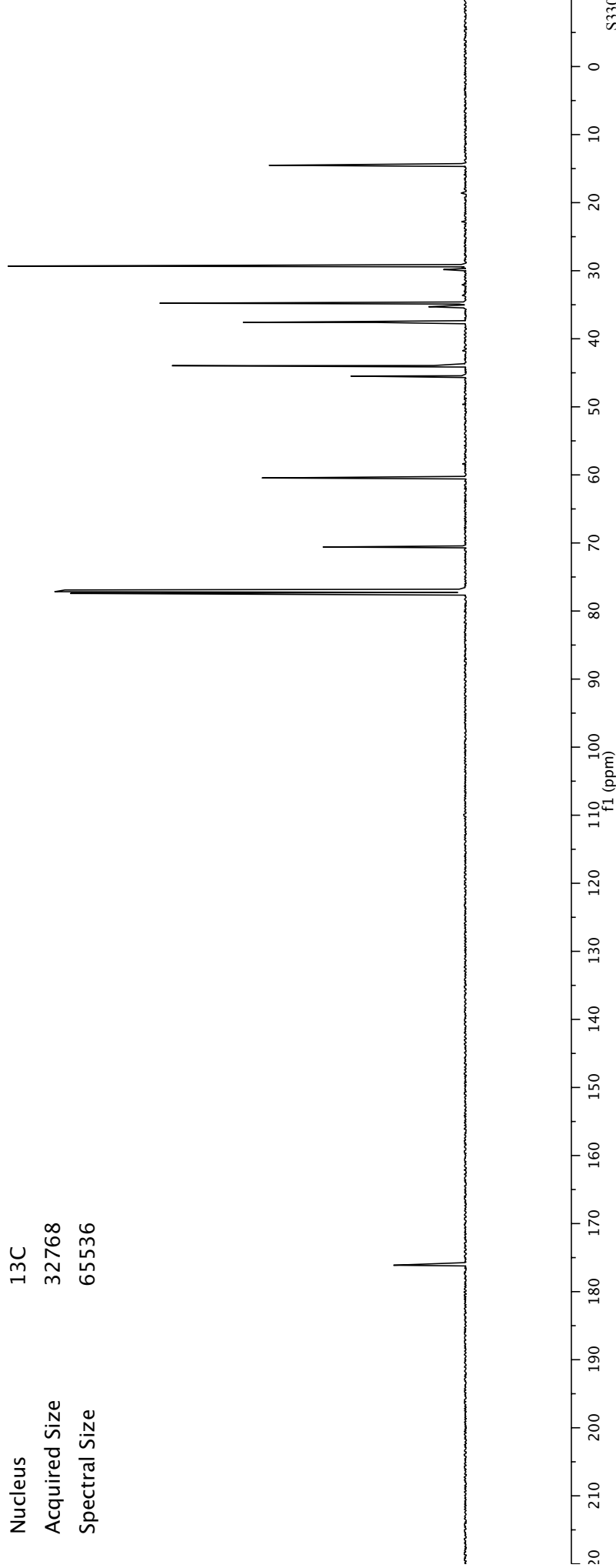


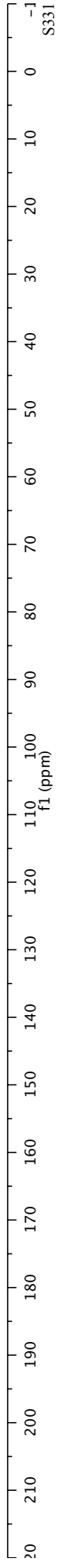
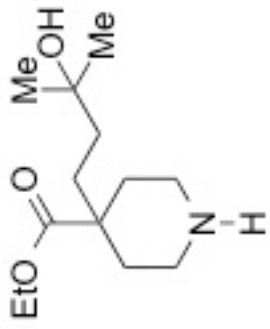
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	28
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1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

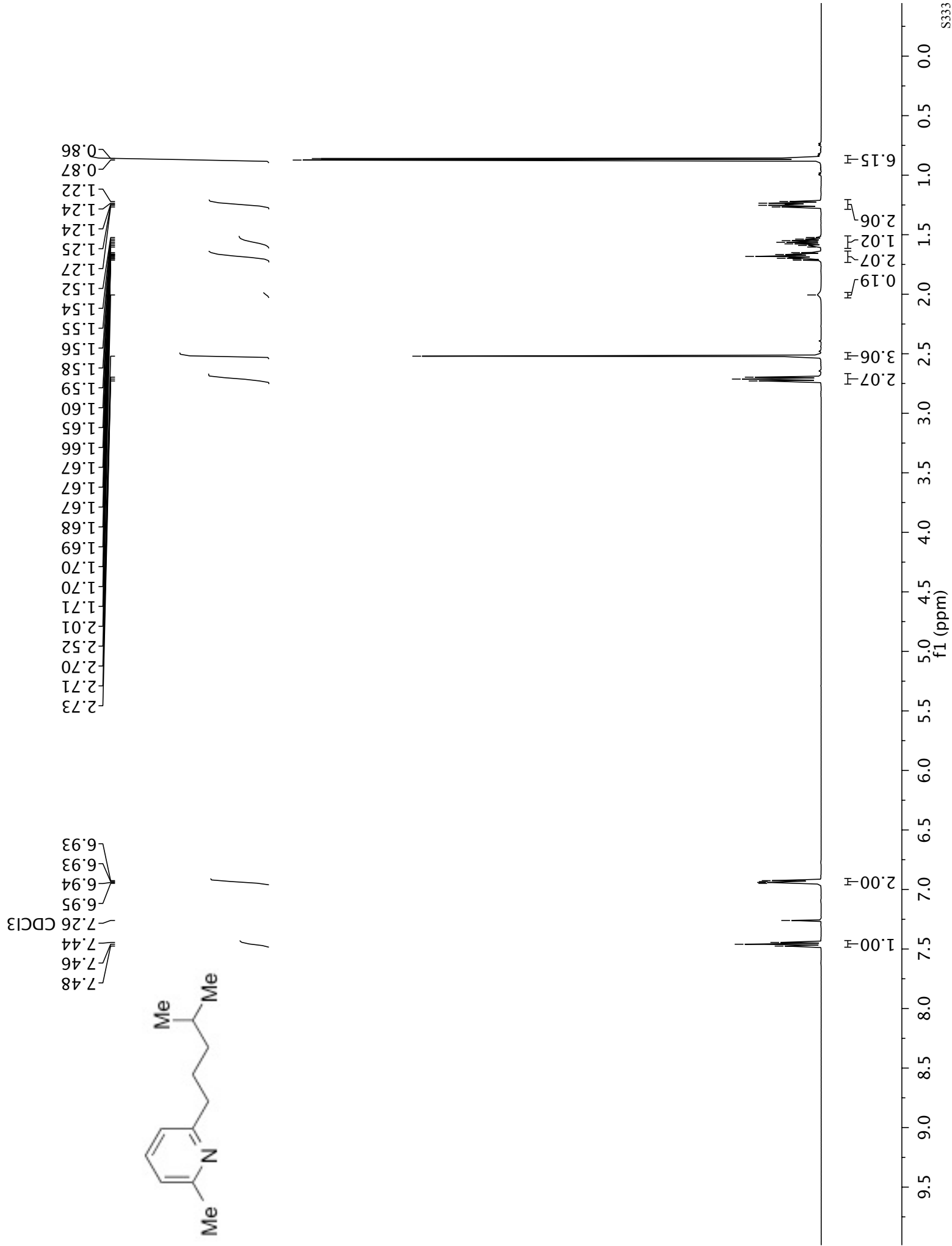


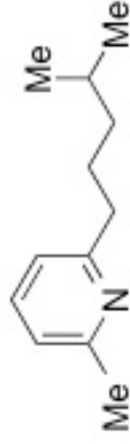


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	11999
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency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

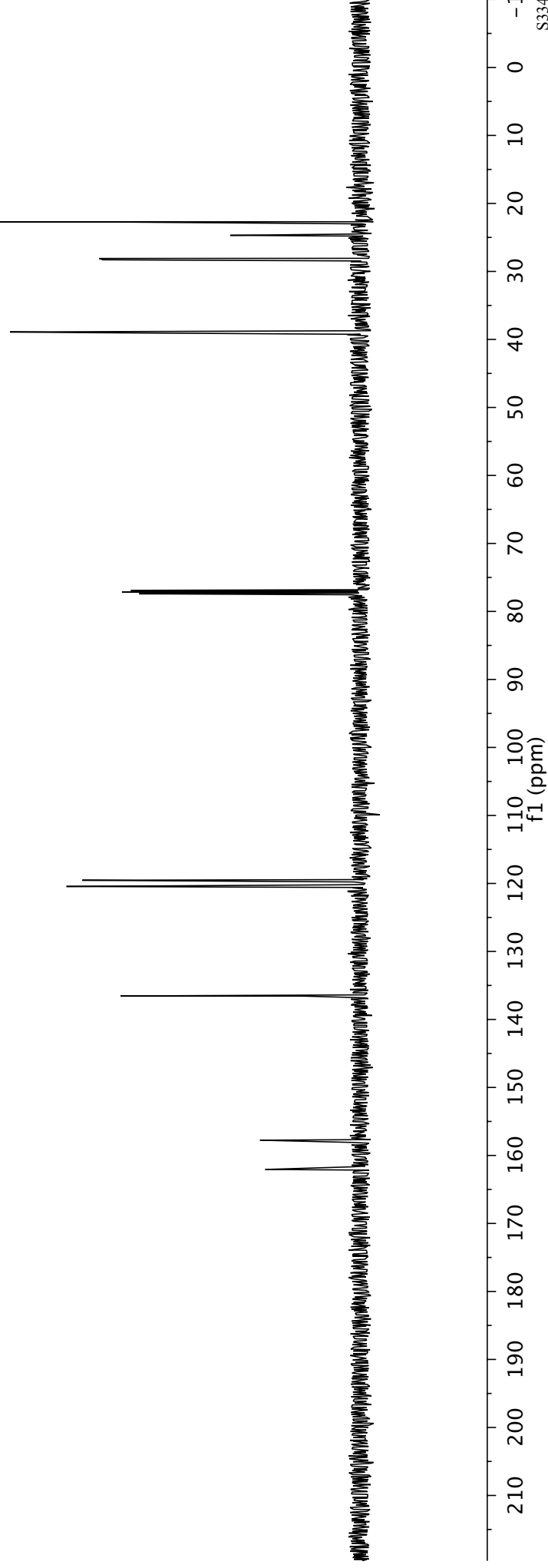


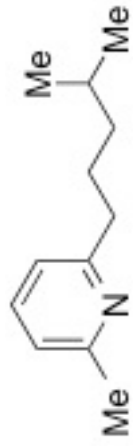






Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1274.8
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536





— 162.07
— 157.77

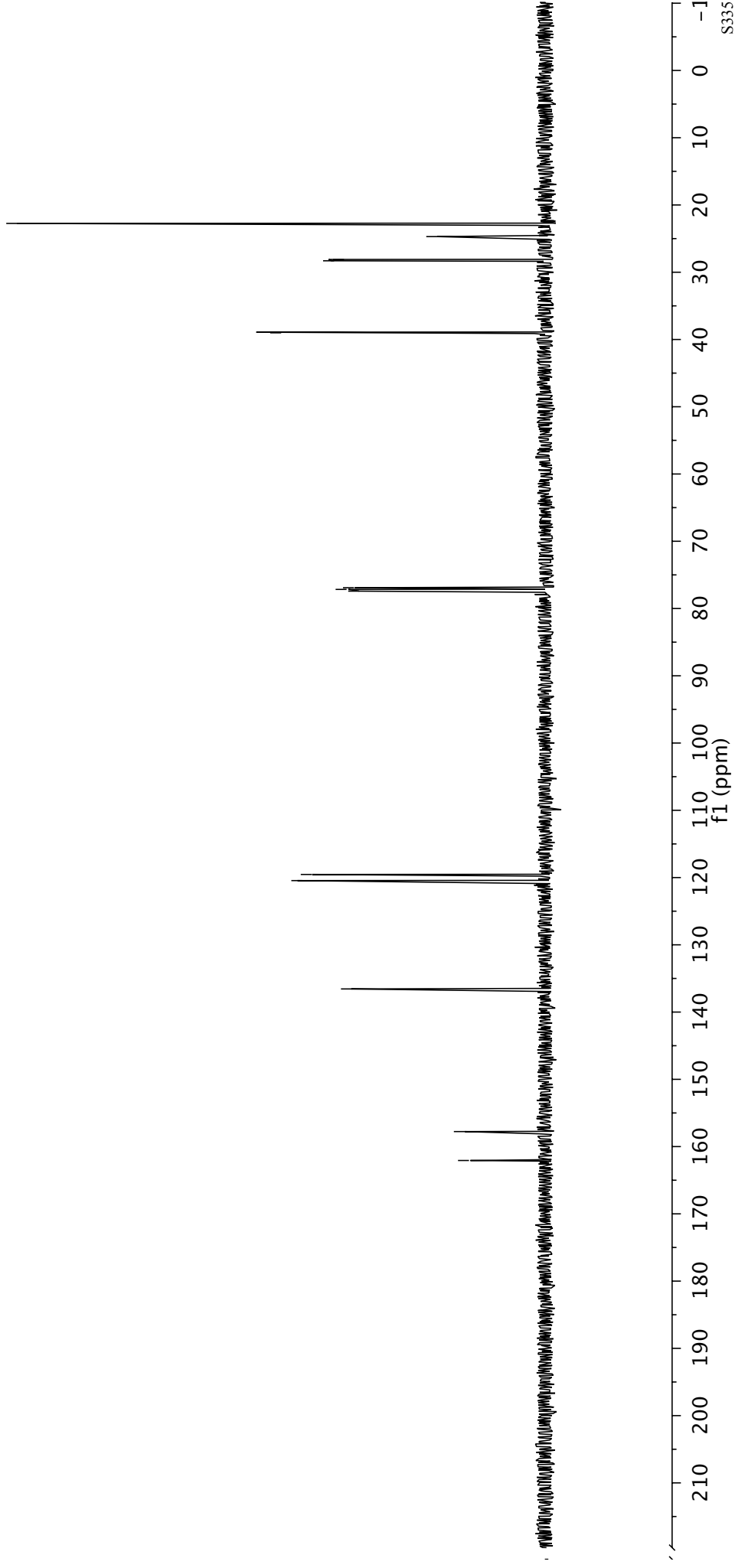
— 136.56

~ 120.45
~ 119.54

77.41 CDCl₃
77.16 CDCl₃
76.91 CDCl₃

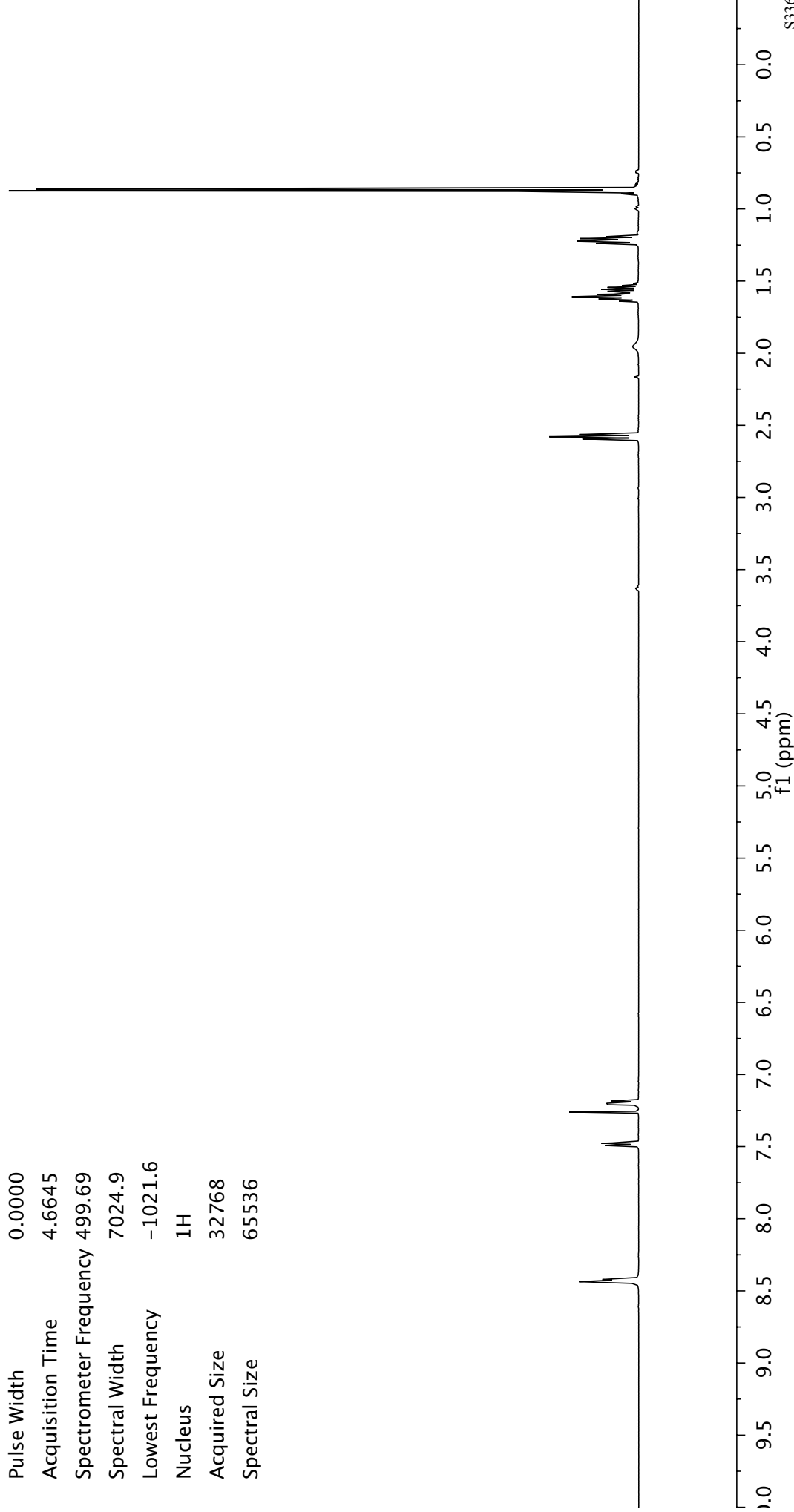
39.01
38.92

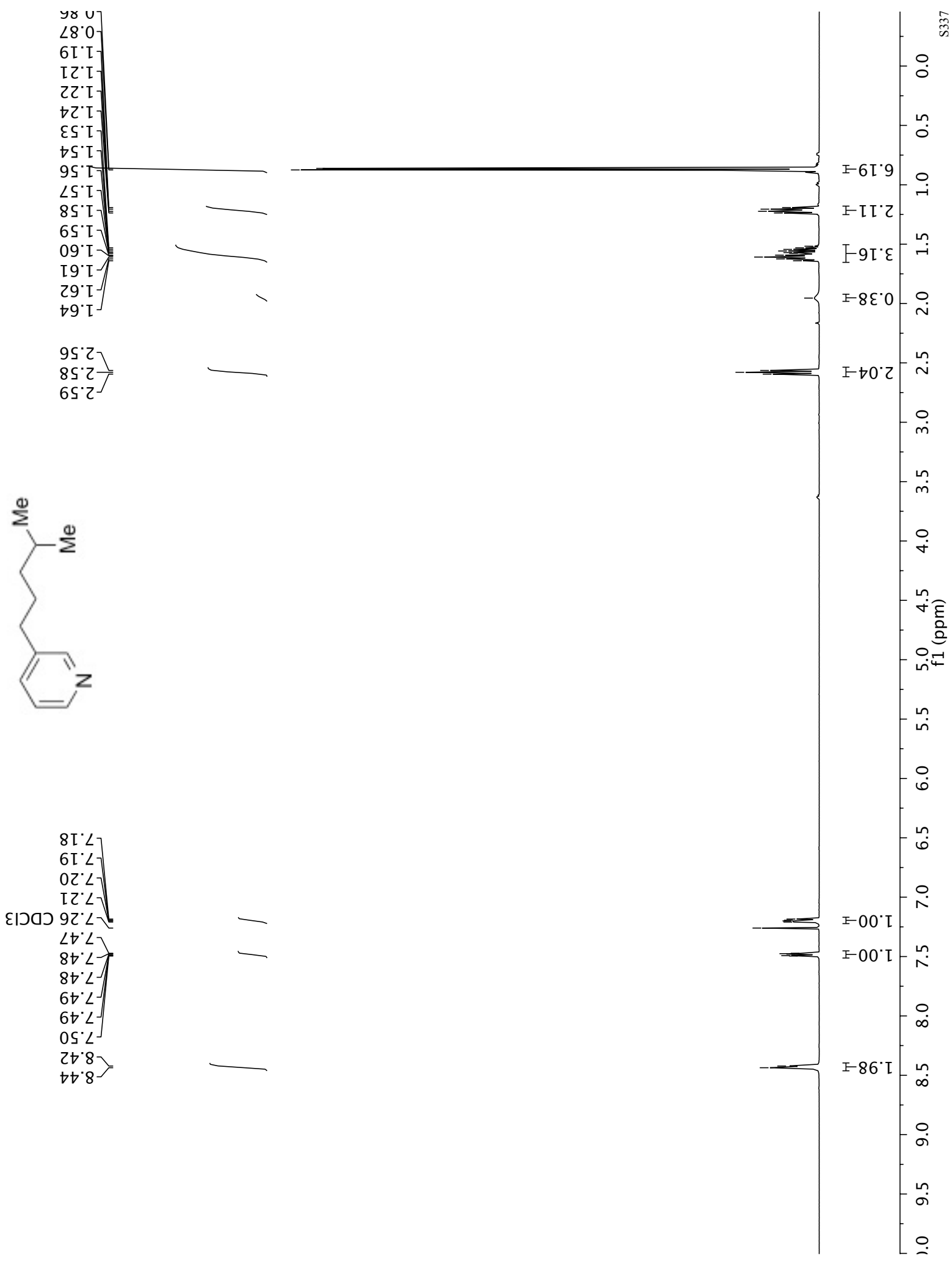
28.30
28.10
24.70
22.74

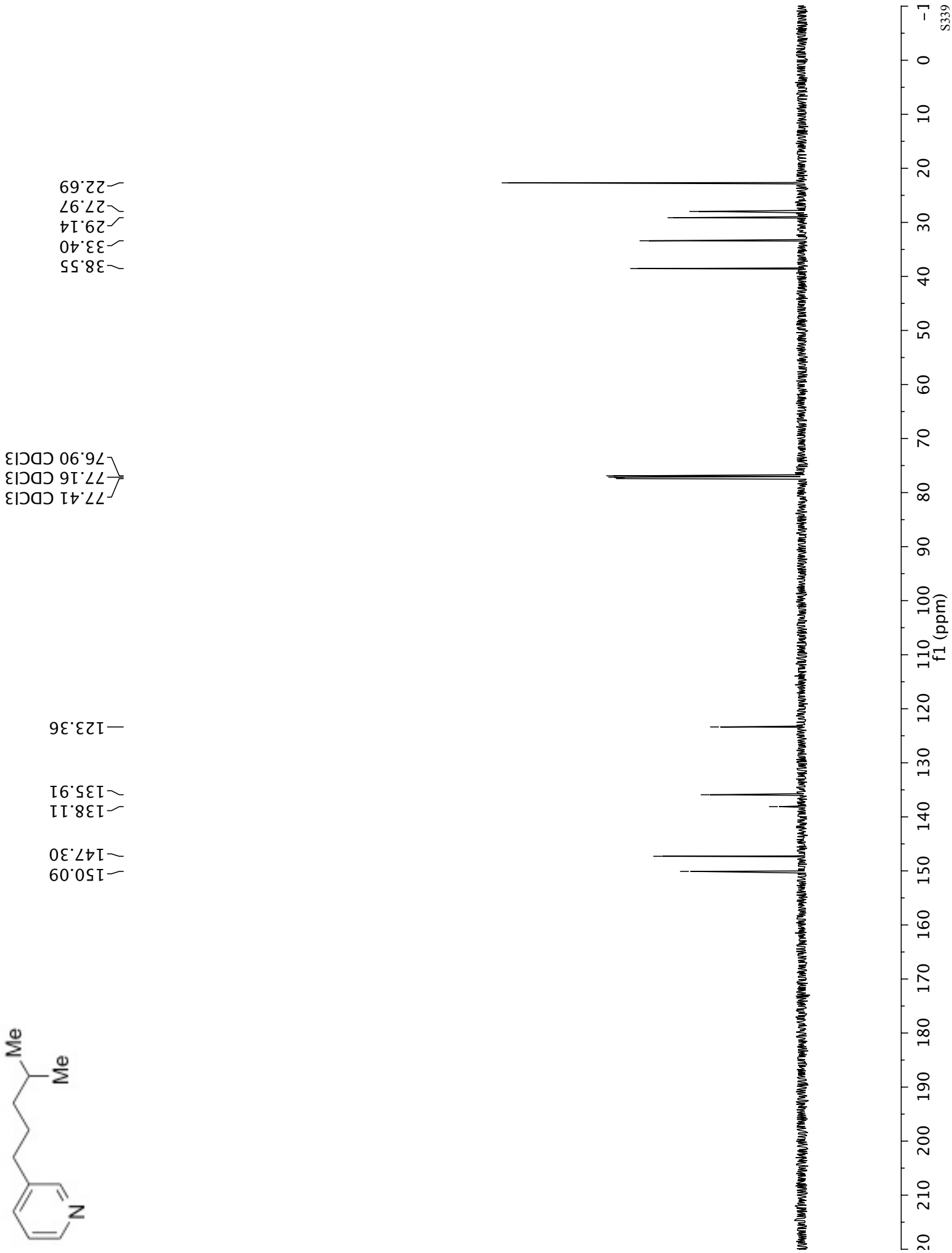


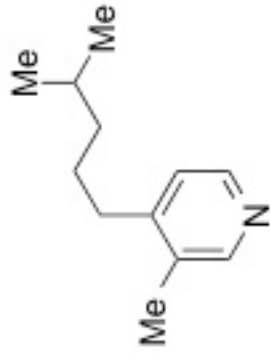


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	46
Relaxation Delay	5.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.69
Spectral Width	7024.9
Lowest Frequency	-1021.6
Nucleus	1H
Acquired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

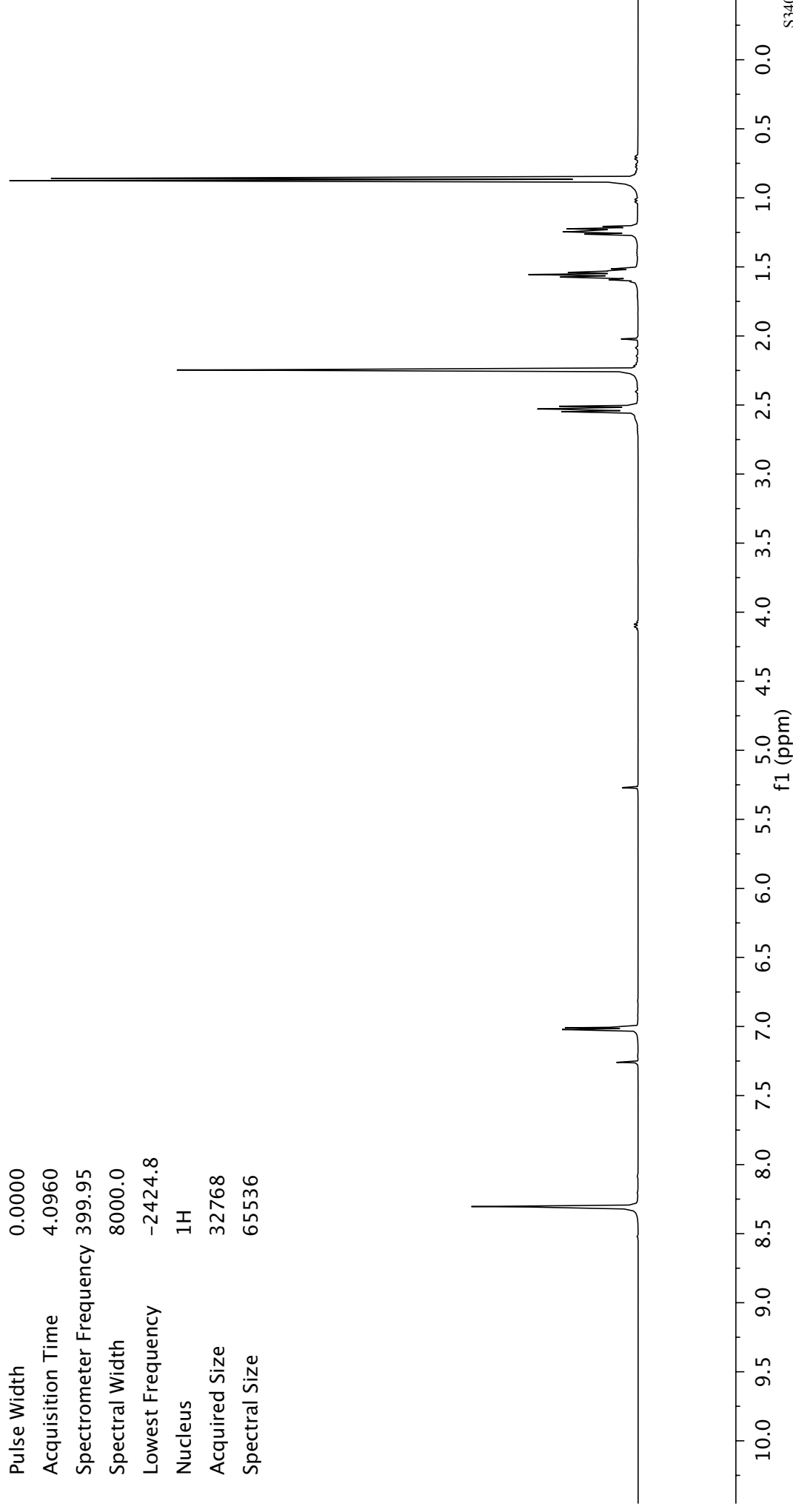


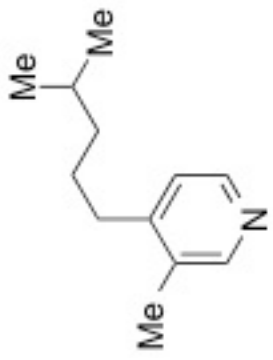






Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	40
Relaxation Delay	5.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	399.95
Spectral Width	8000.0
Lowest Frequency	-2424.8
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

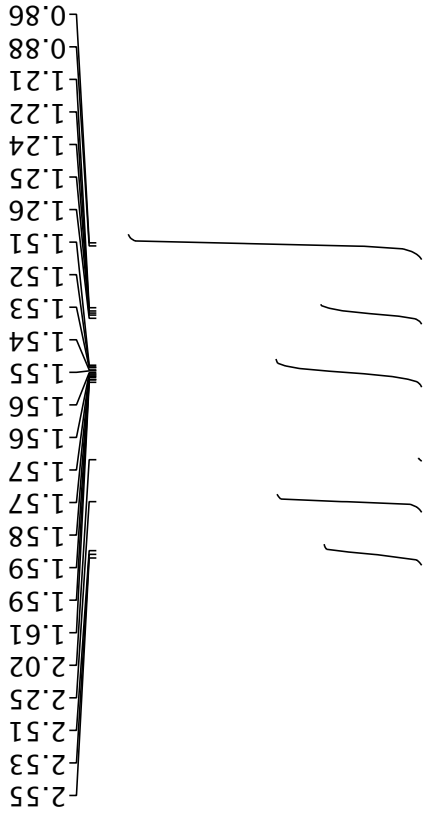




7.26 CDCl₃
7.02
7.01

8.31
8.30

-5.27



0.05

1.01

1.92

6.33

2.17

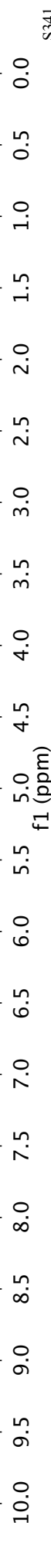
3.14

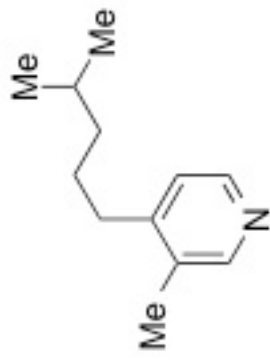
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3.12

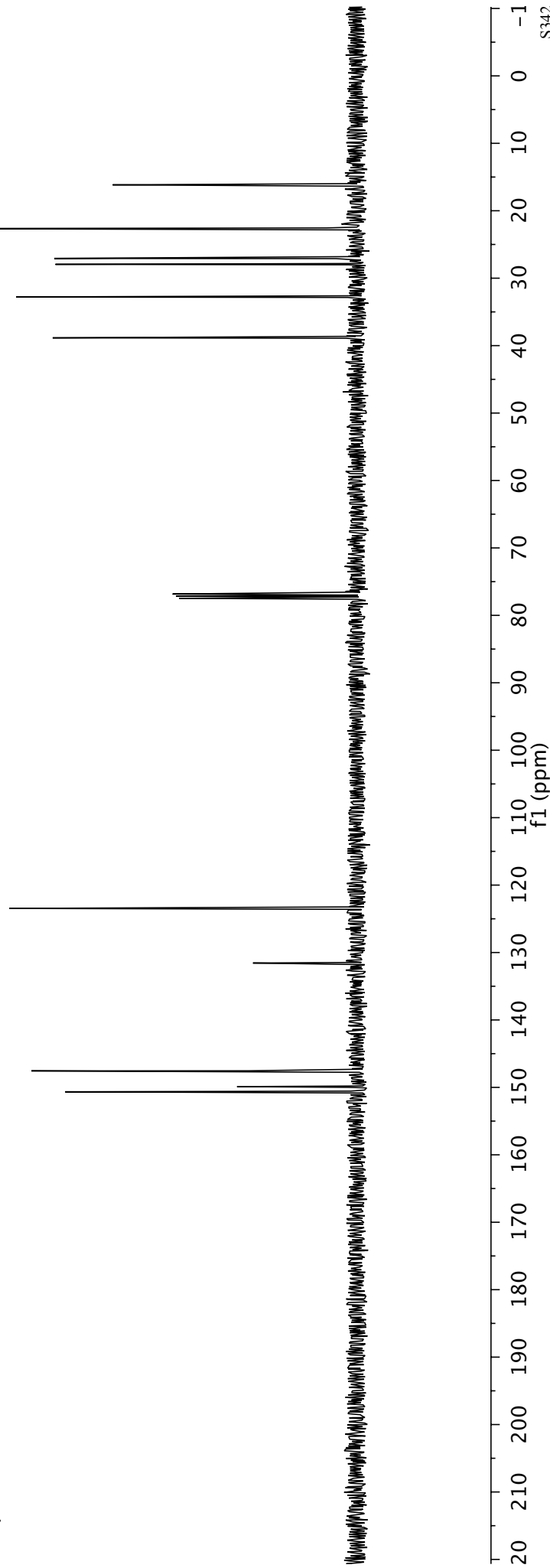
2.10

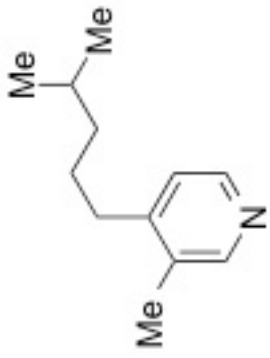
f1 (ppm)





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	-1029.5
Nucleus	13C
Acquired Size	32768
Spectral Size	65536





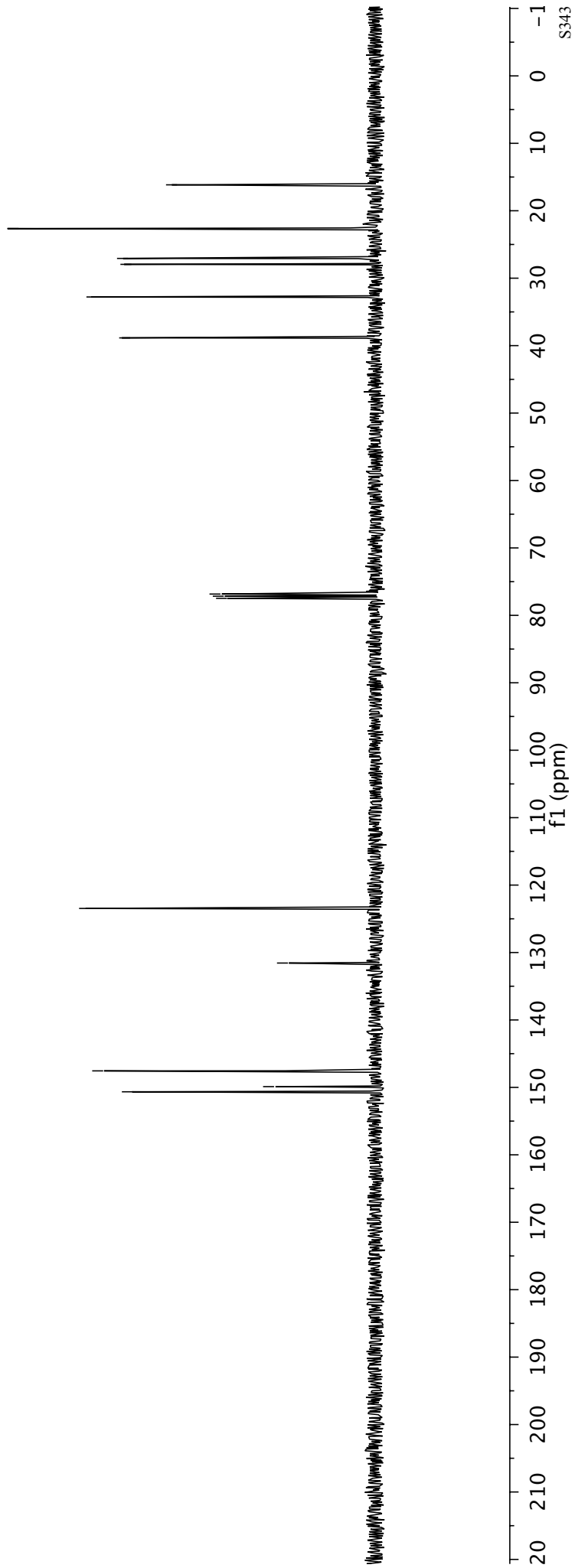
38.85
 32.78
 27.95
 27.07
 22.64
 16.16

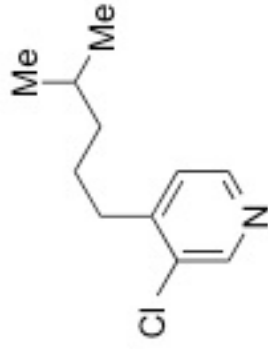
77.48 CDCl₃
 77.16 CDCl₃
 76.84 CDCl₃

123.46

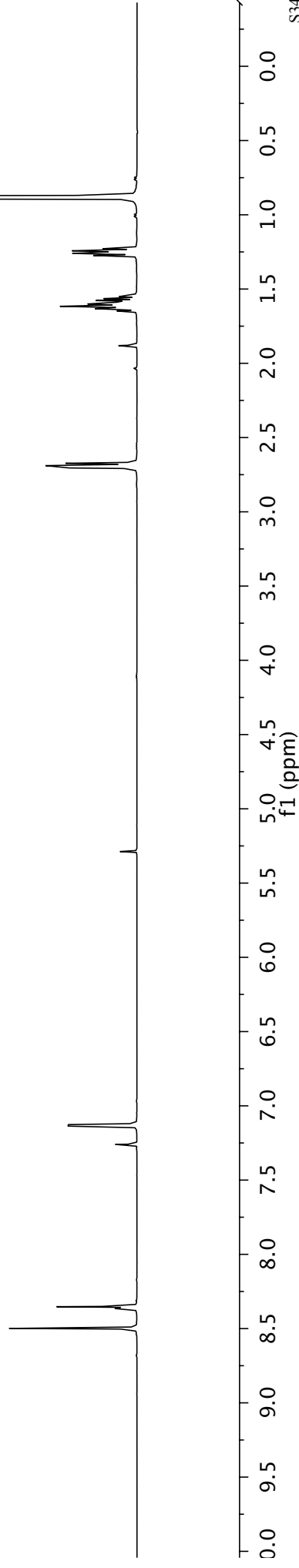
131.56

150.66
 149.89
 147.55

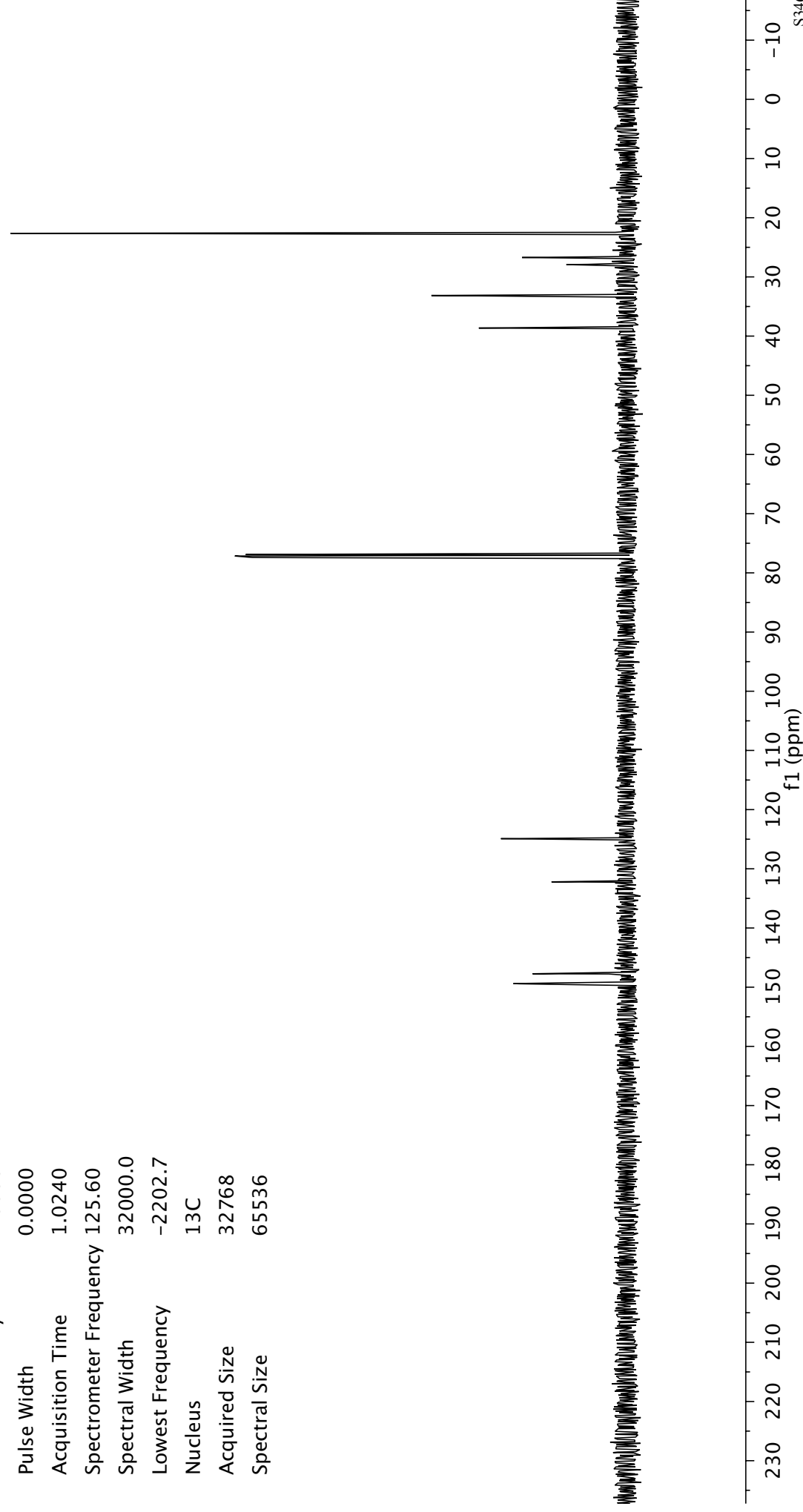
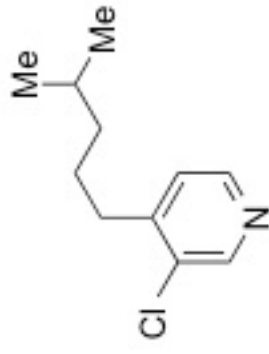


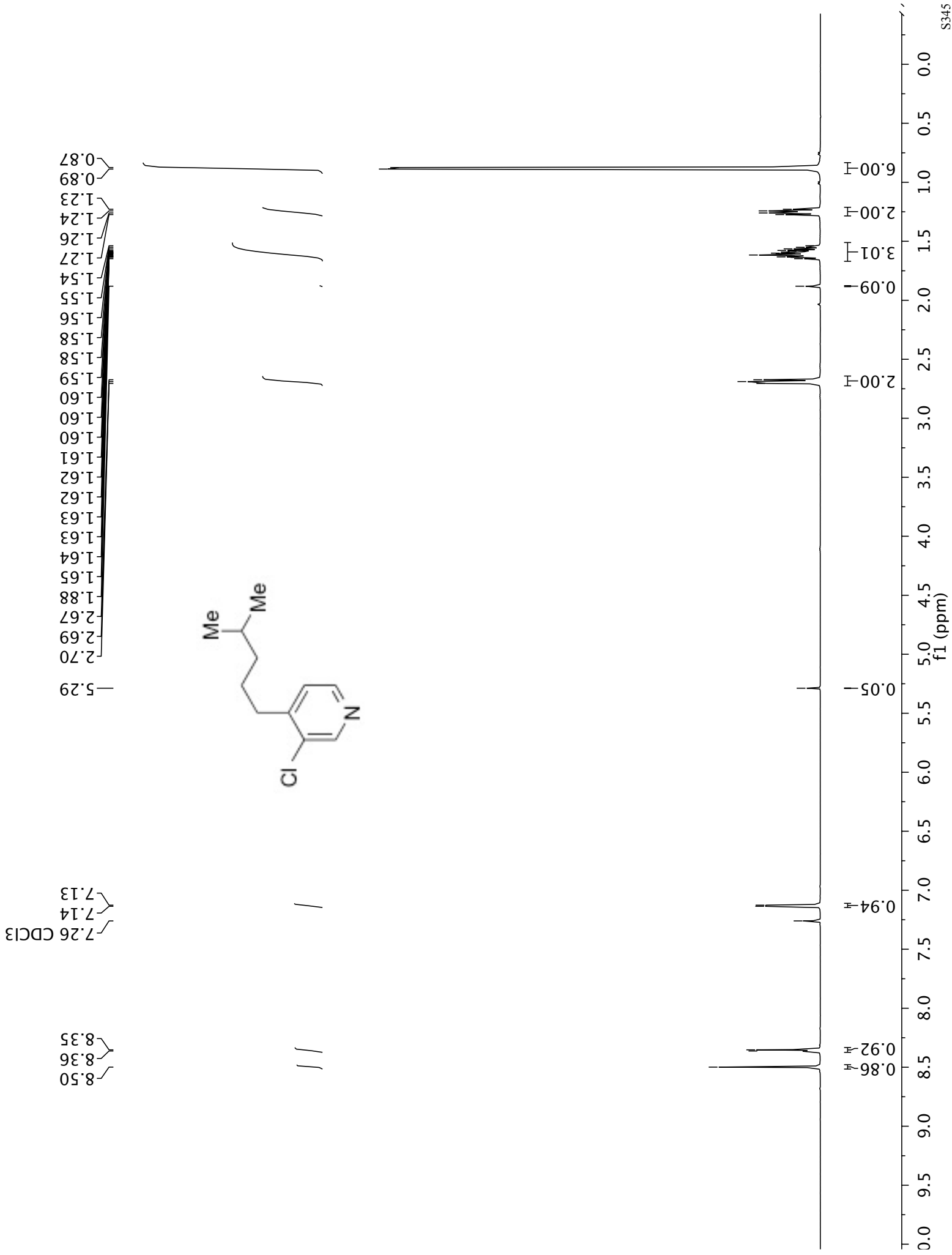


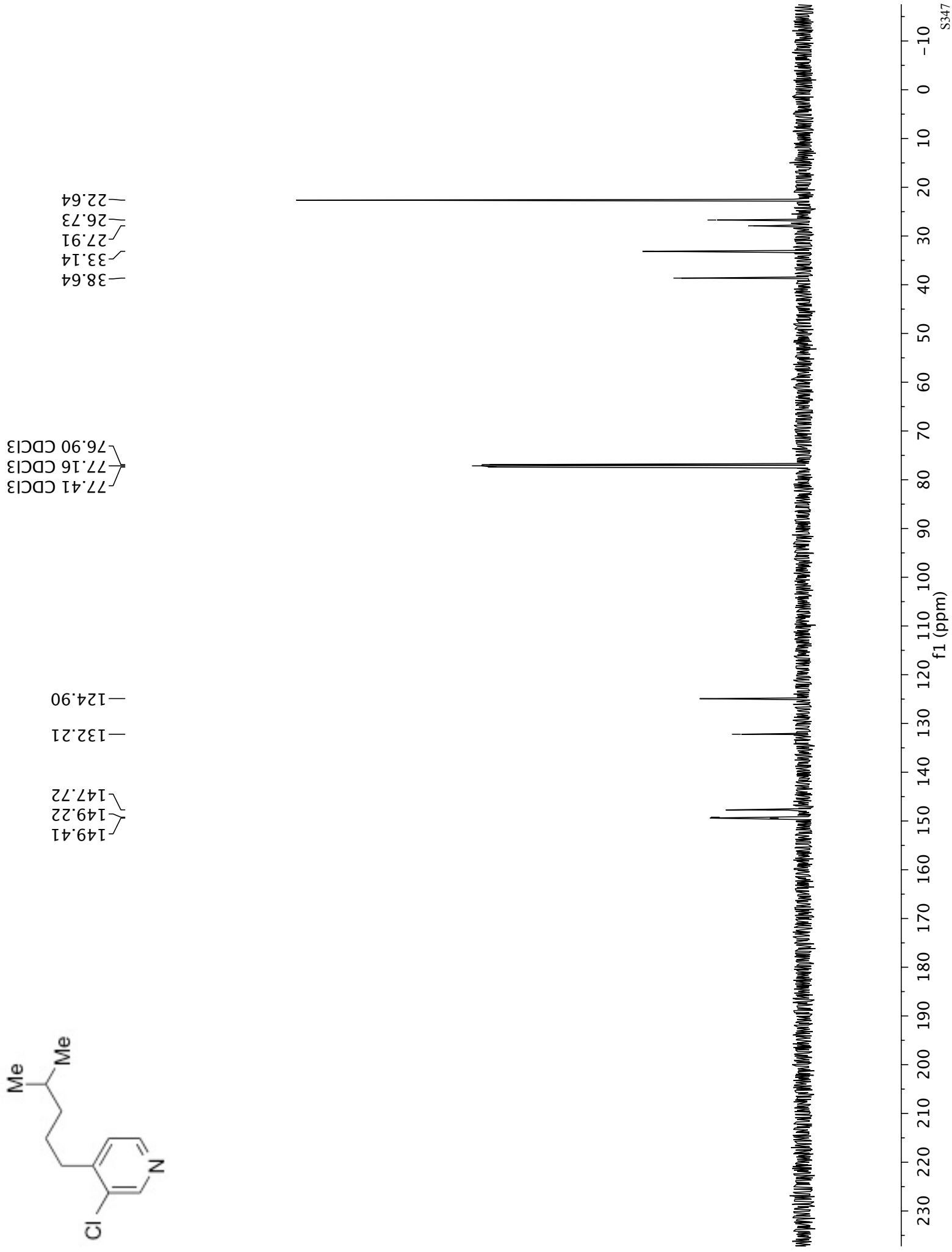
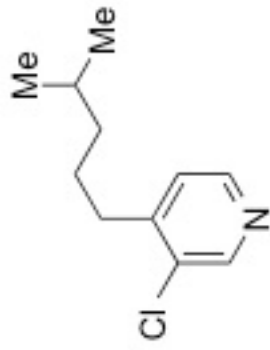
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	26
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

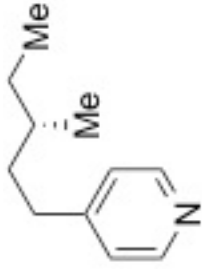


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2202.7
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

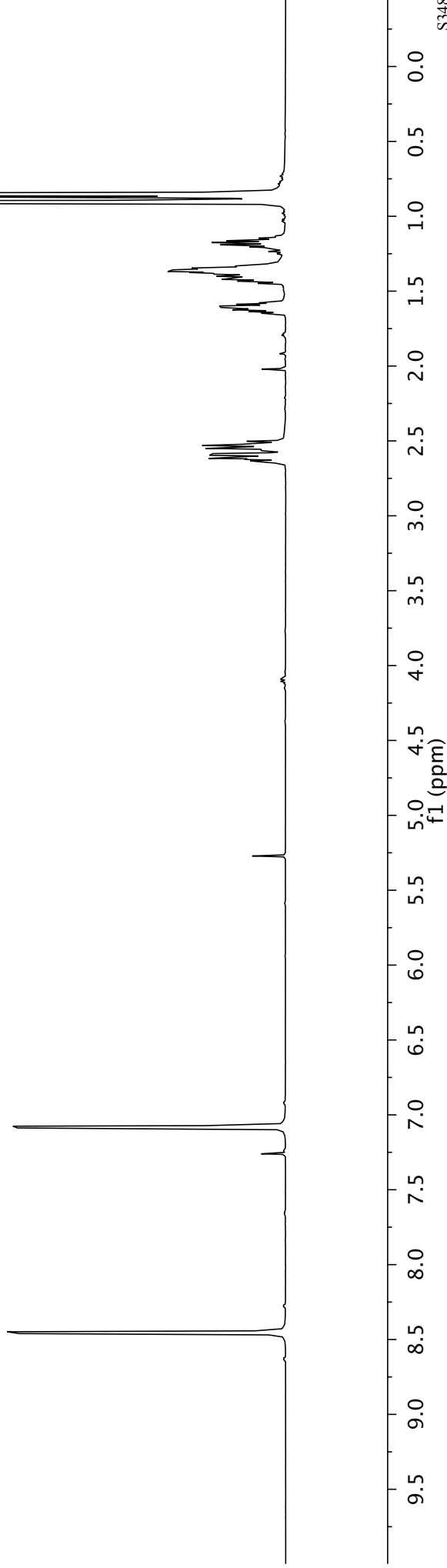


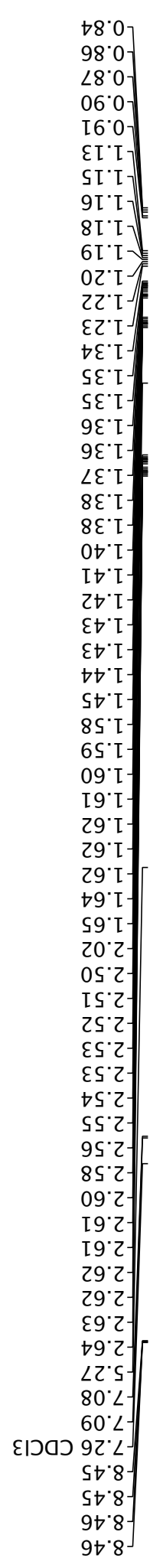
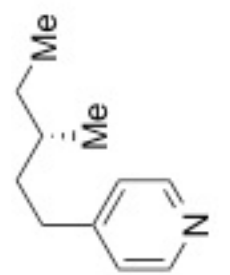
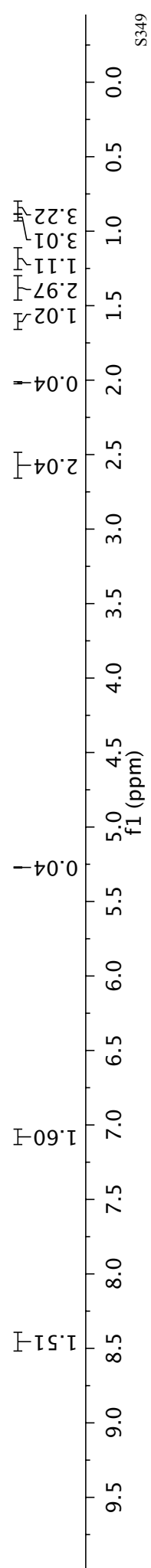




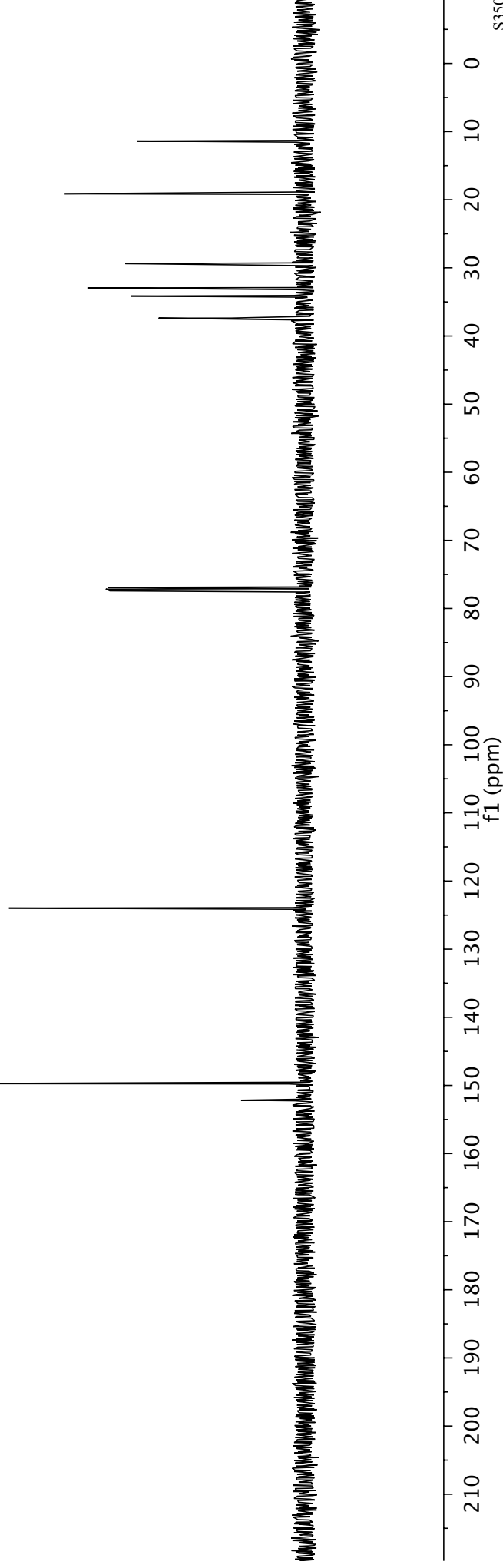
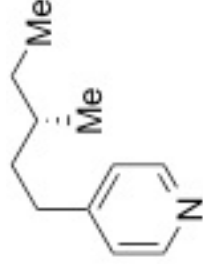


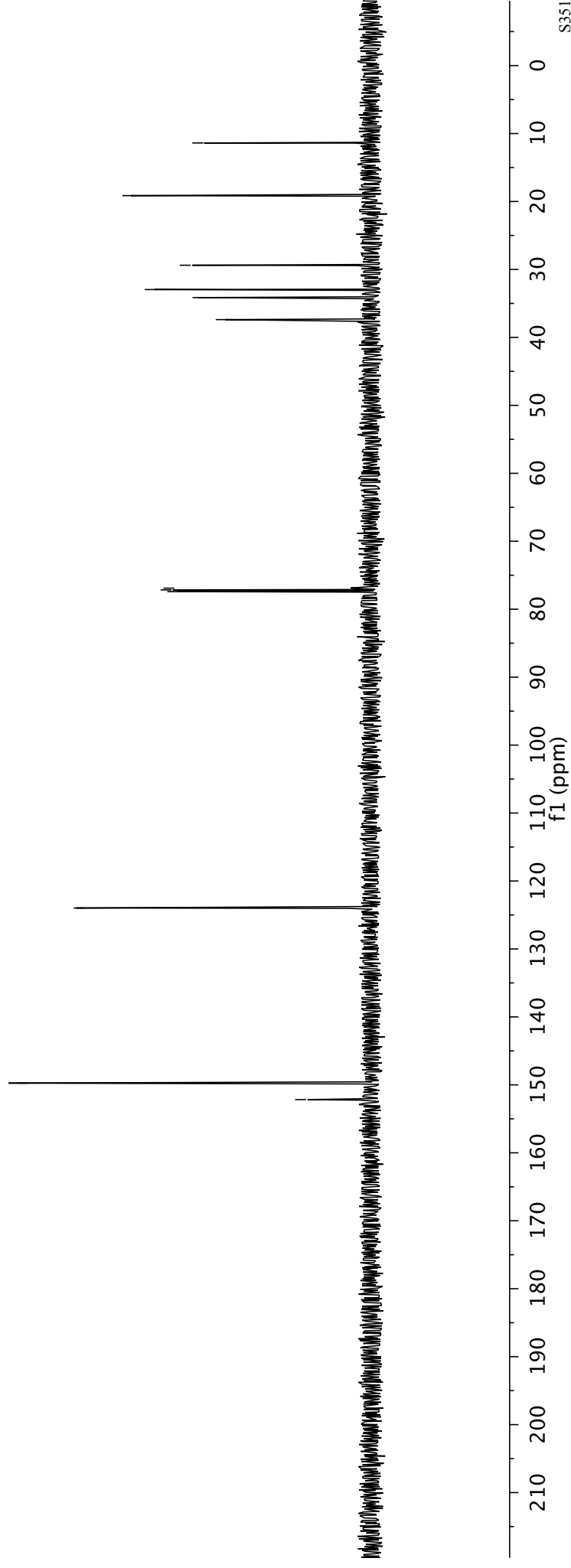
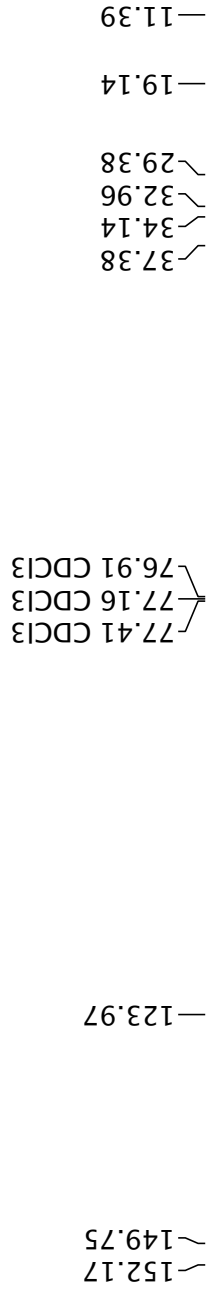
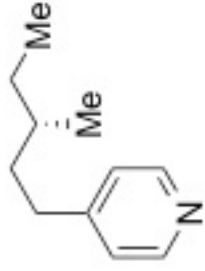
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	22
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1510.9
Nucleus	1H
Acquired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

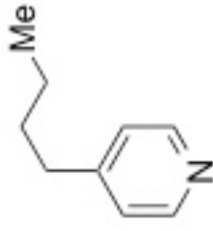




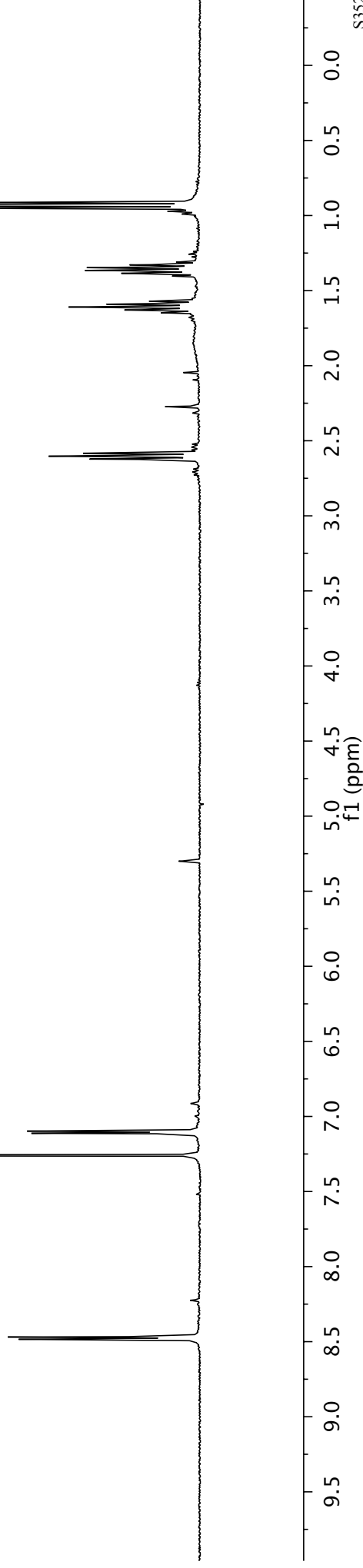
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2204.6
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

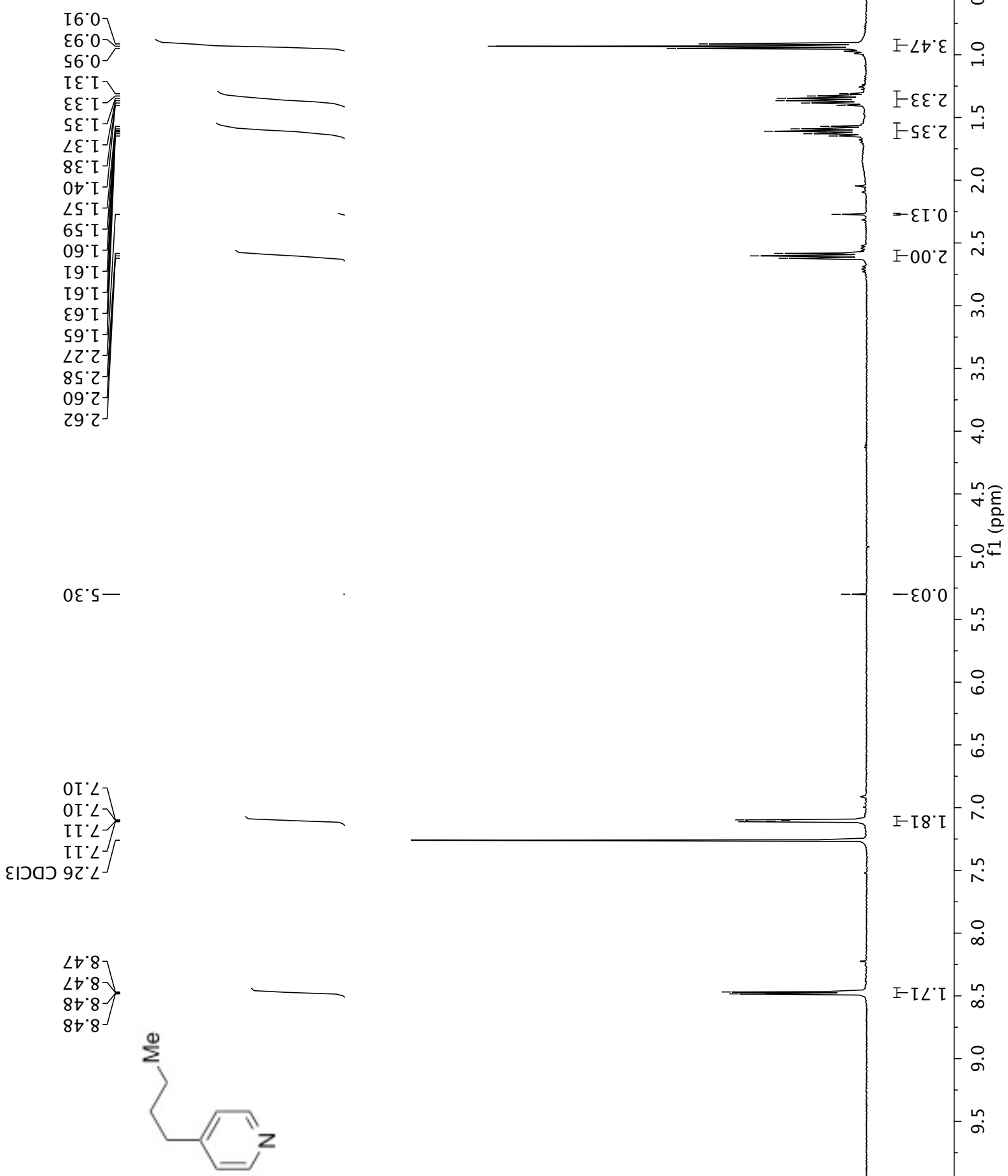


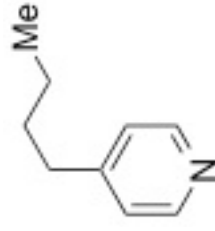




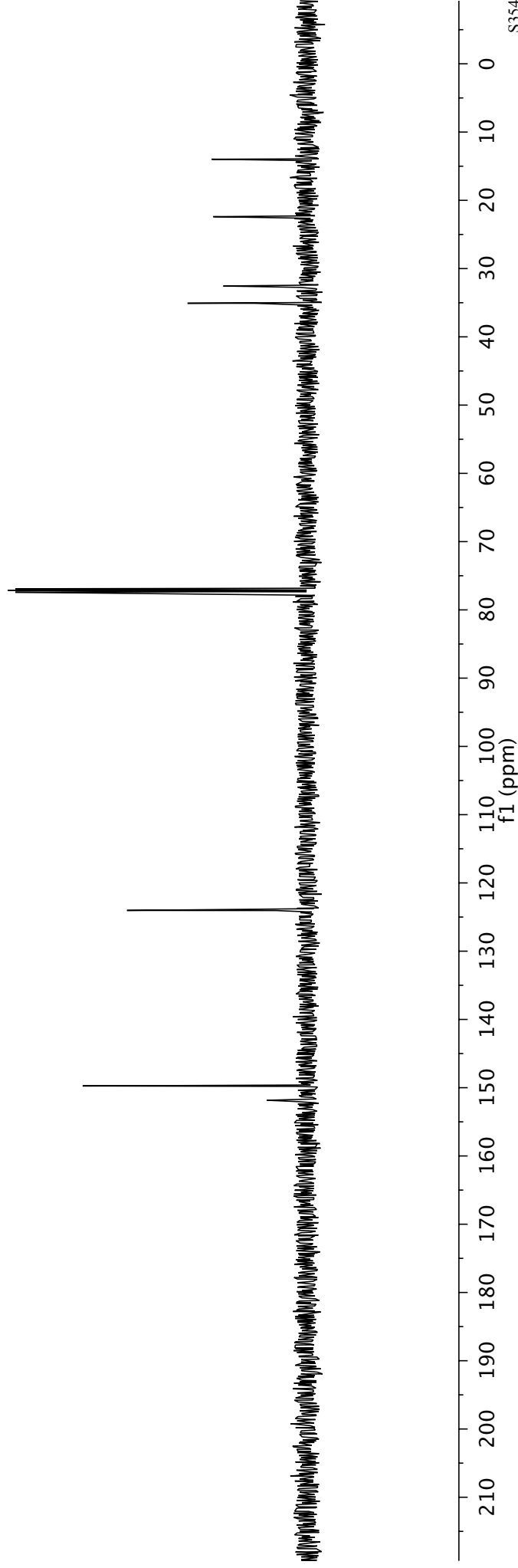
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	399.95
Spectral Width	8000.0
Lowest Frequency	-2424.5
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

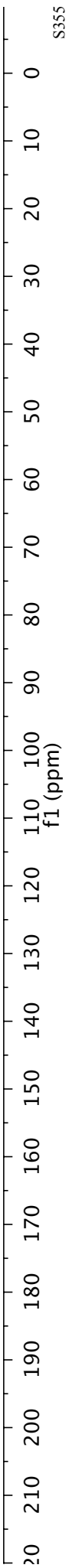
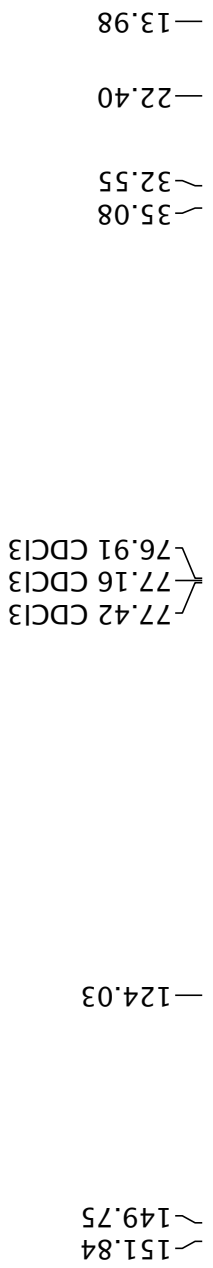
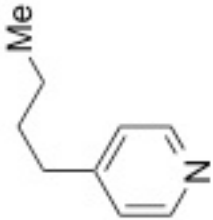


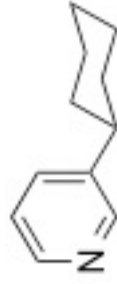




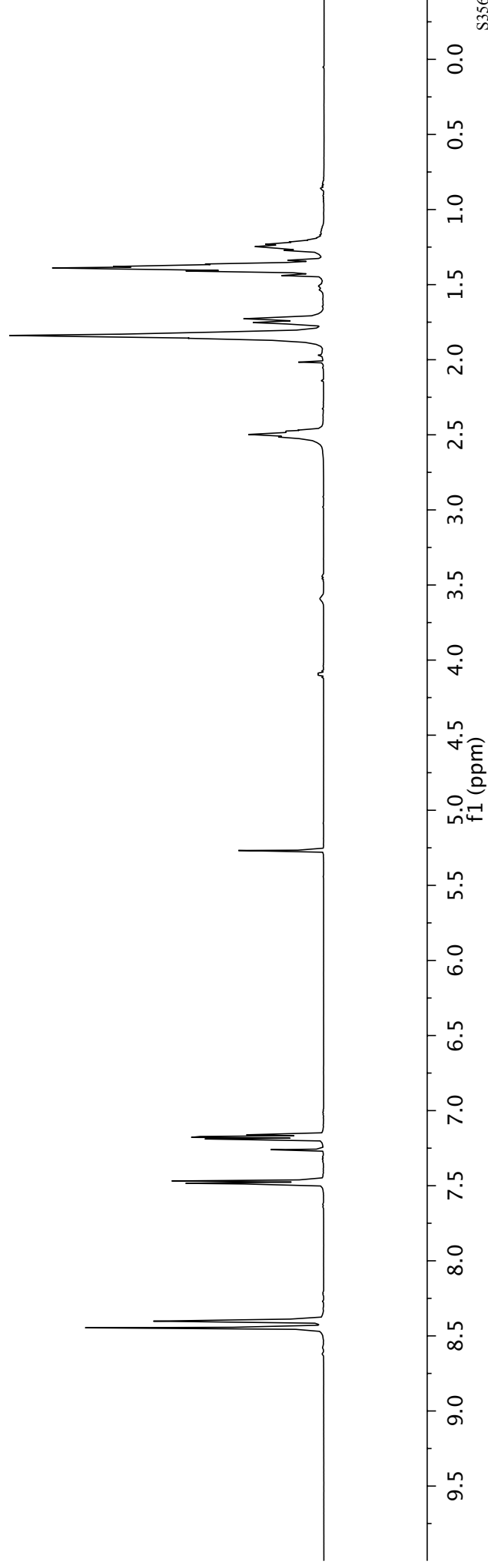
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2199.3
Nucleus	¹³ C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

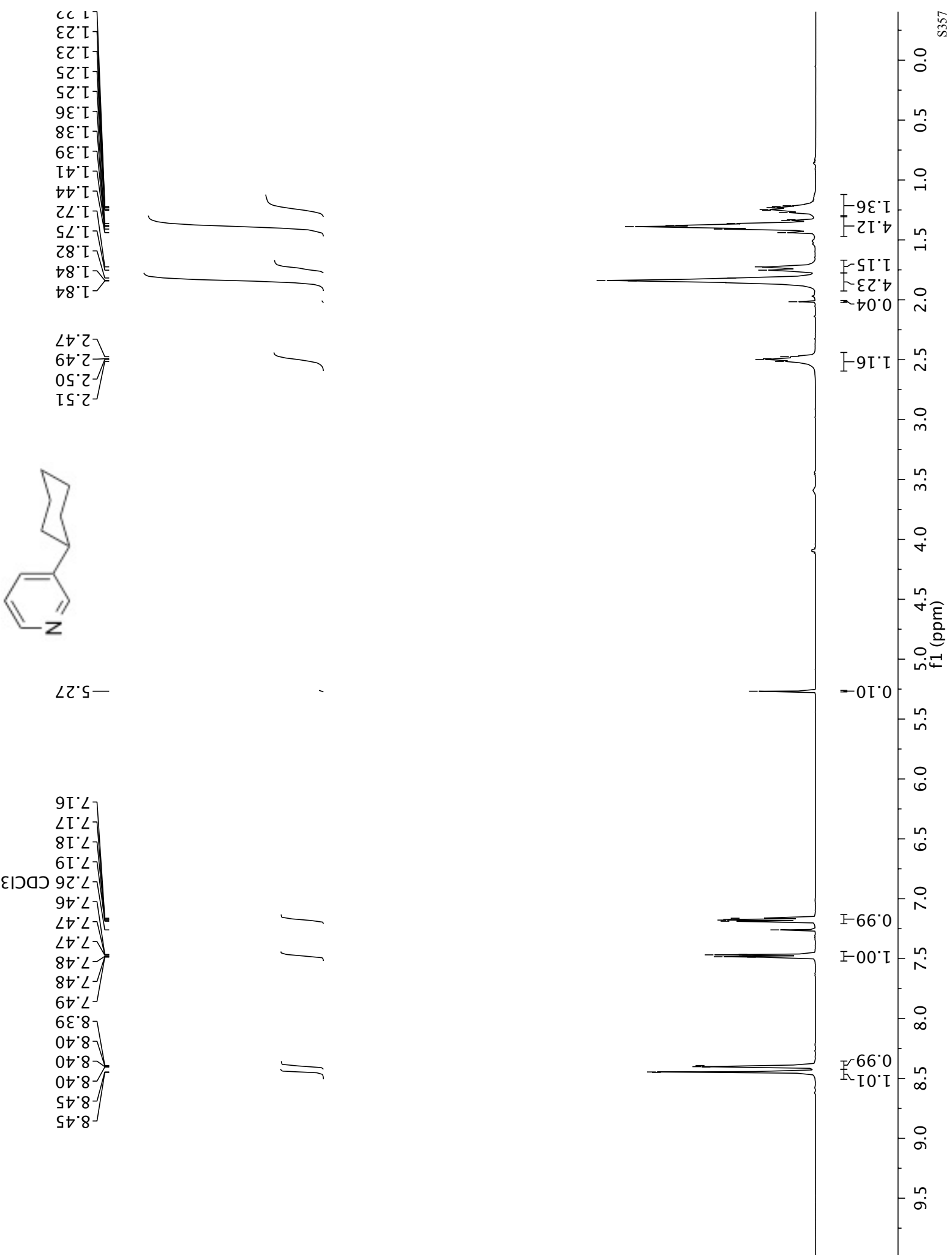






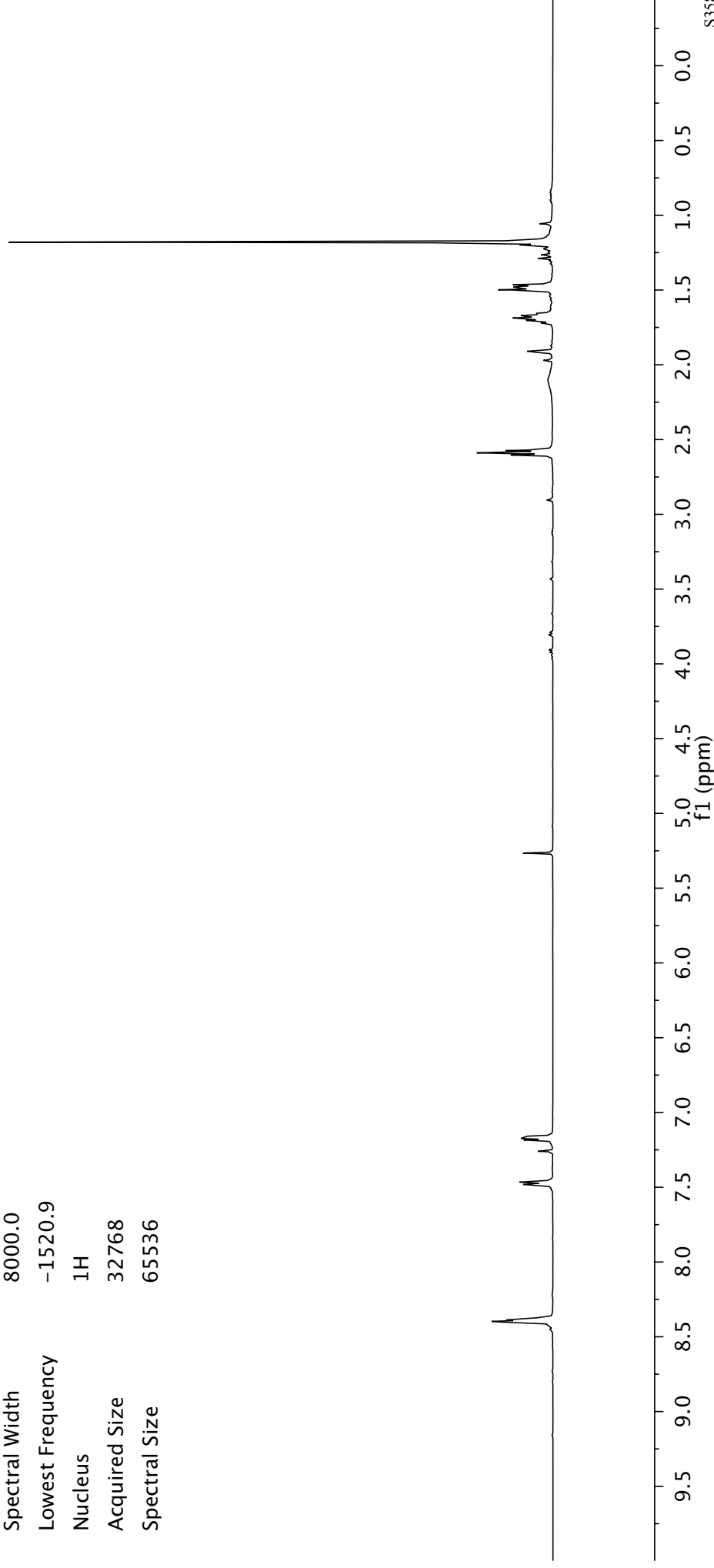
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	22
Relaxation Delay	15.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	¹ H
Acquired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

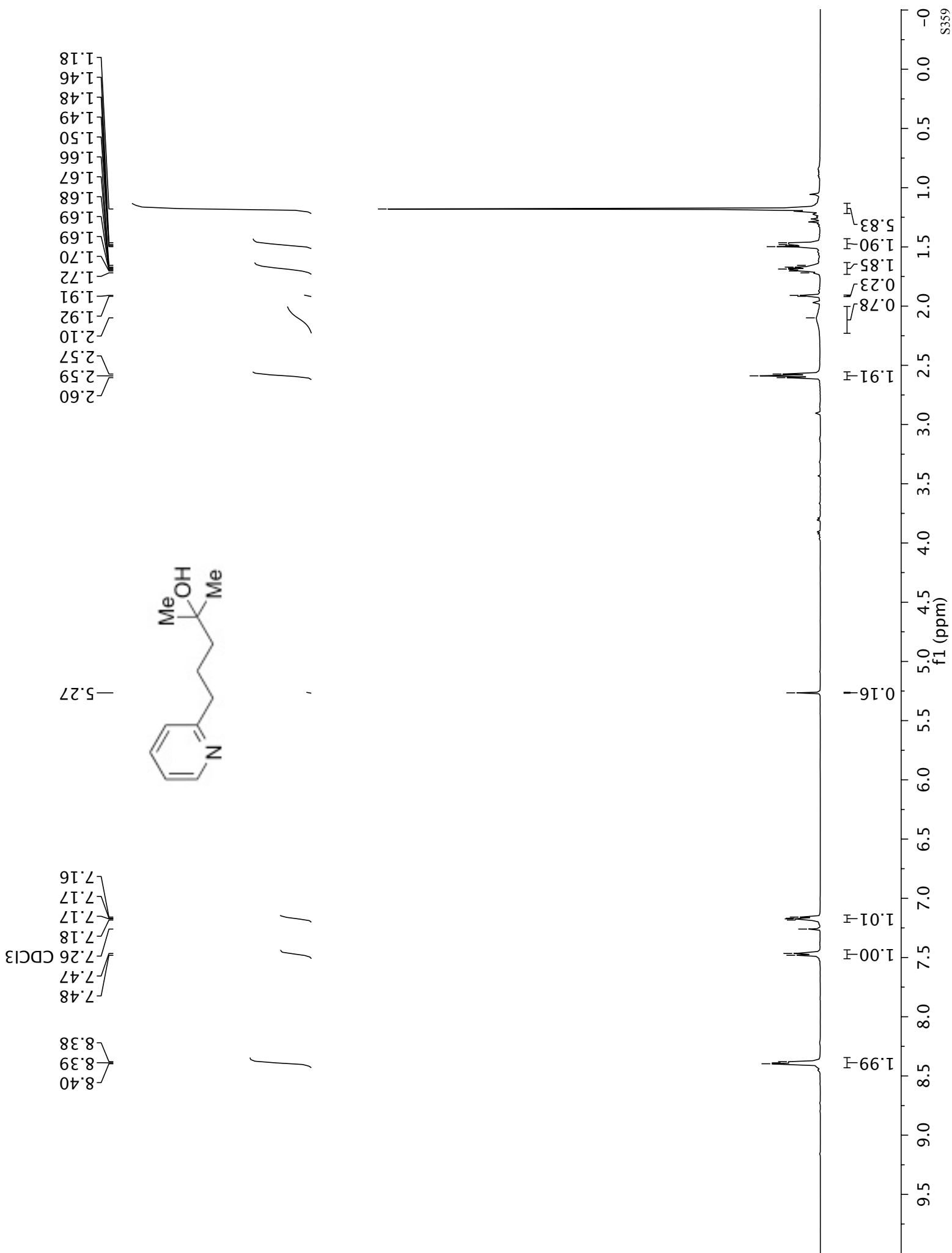






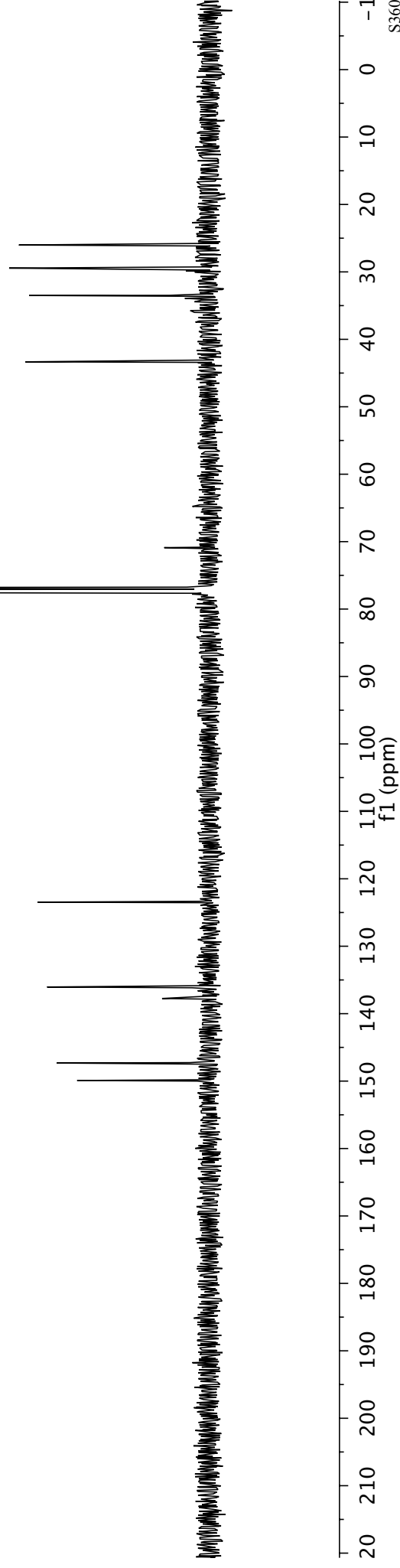
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	22
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1520.9
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

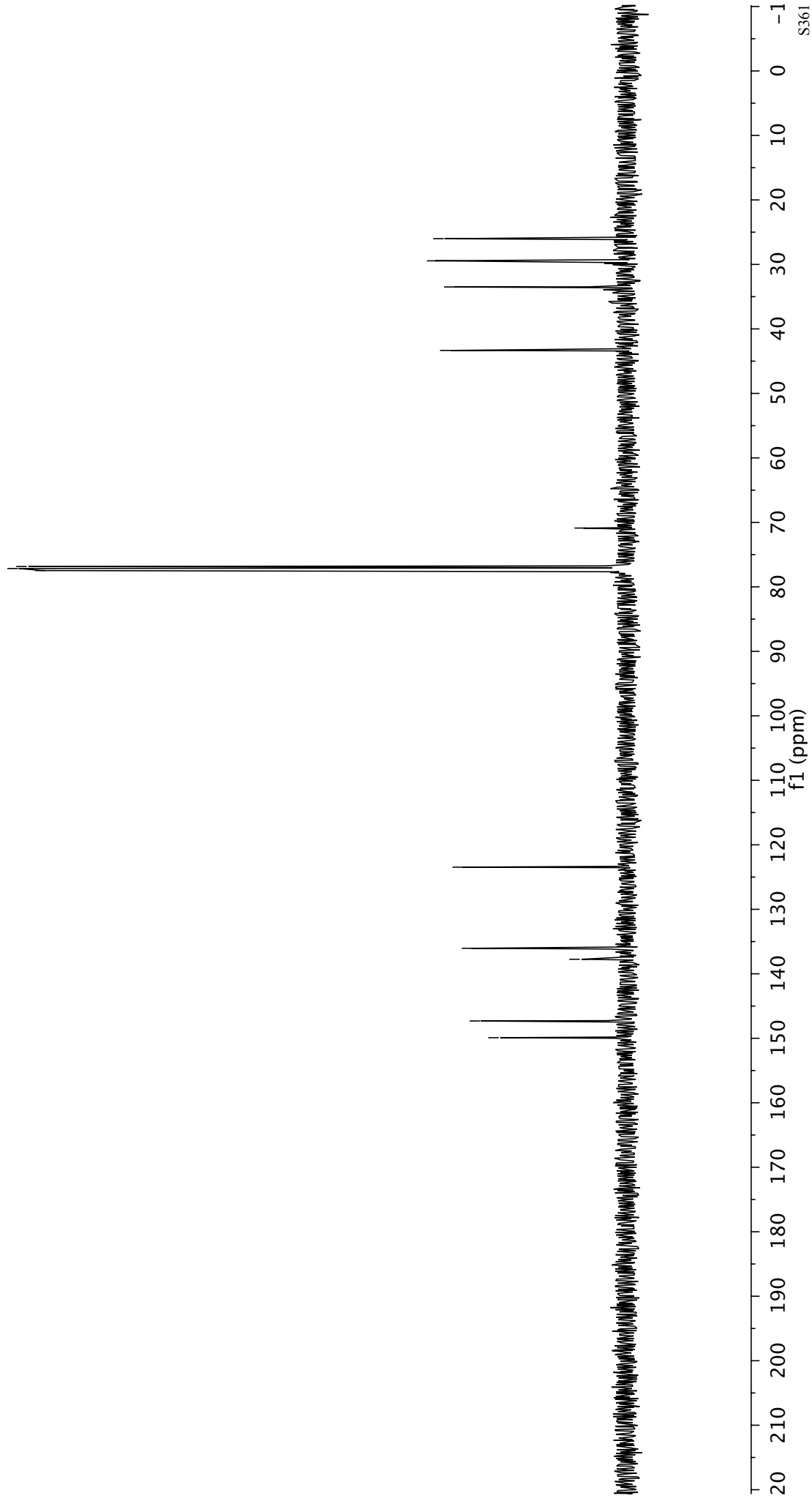
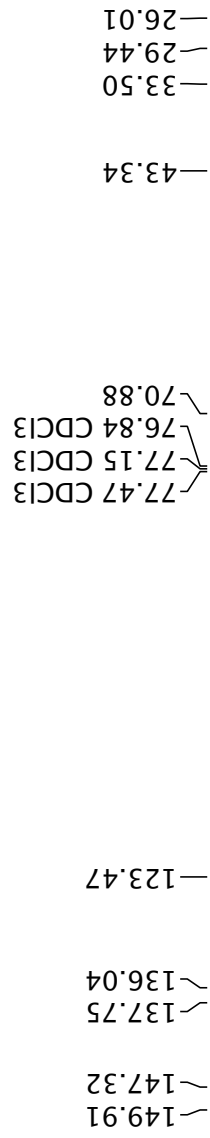


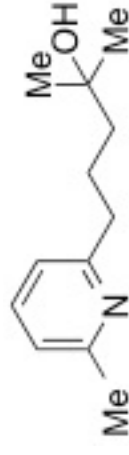




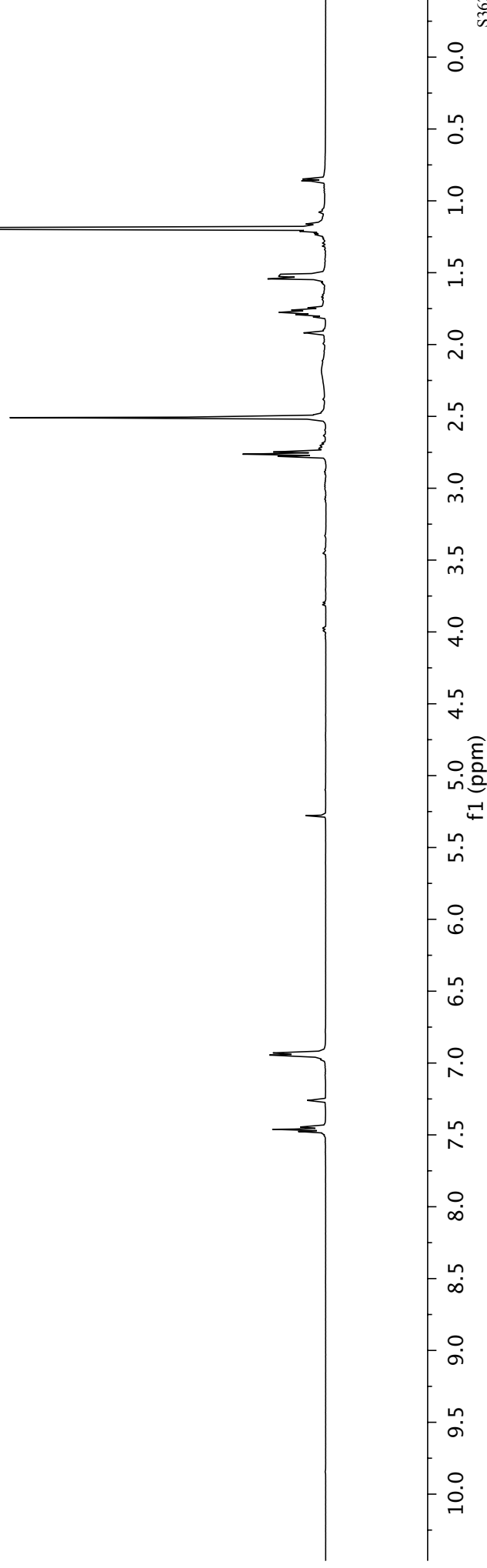
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3107
Spectrometer Frequency	100.58
Spectral Width	25000.0
Lowest Frequency	-1027.1
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

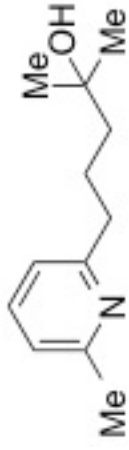






Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	41
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.6645
Spectrometer Frequency	499.69
Spectral Width	7024.9
Lowest Frequency	-1021.6
Nucleus	¹ H
Acquired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





7.48
7.46
7.45
7.26 CDCl₃
6.95
6.94
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

1.00 ±

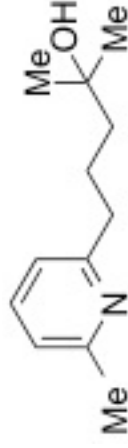
2.01 ±

0.11 ±

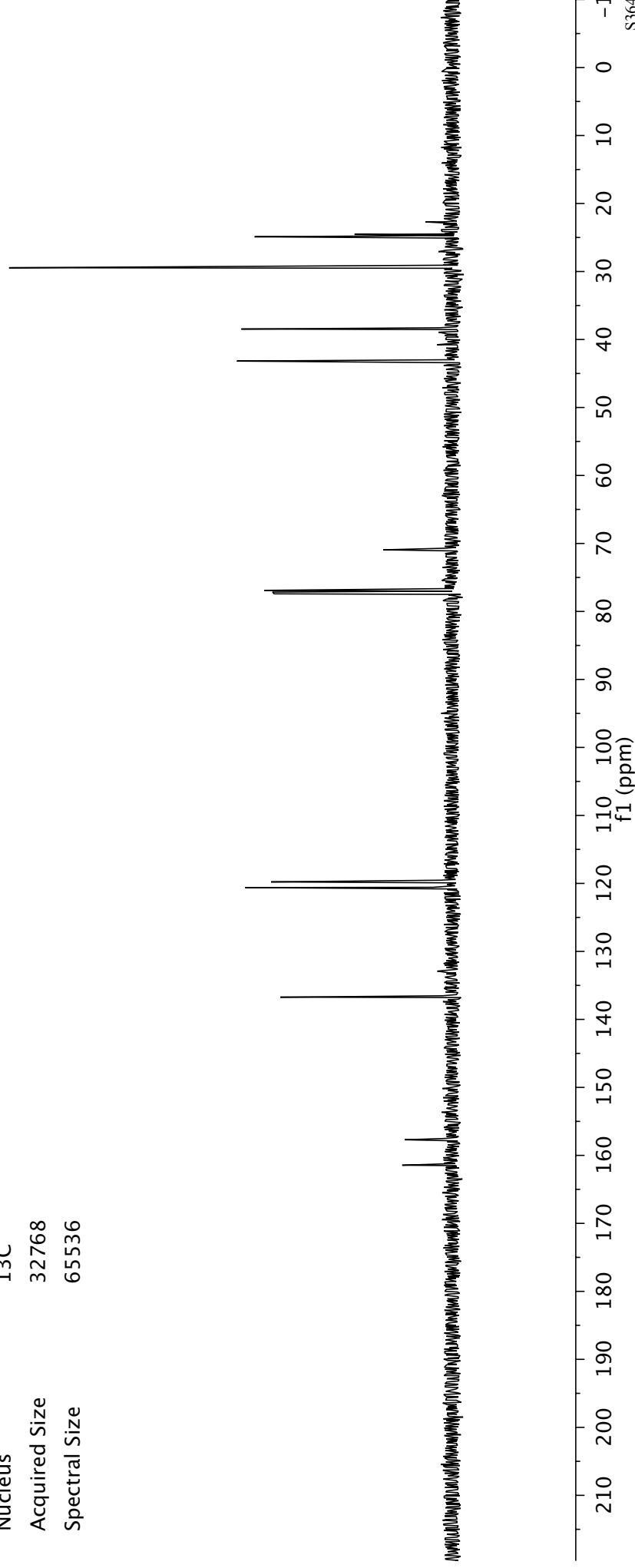
1.94 ±
3.24 ±
0.97 ±
0.17 ±
1.86 ±
1.99 ±
6.24 ±
0.33 ±

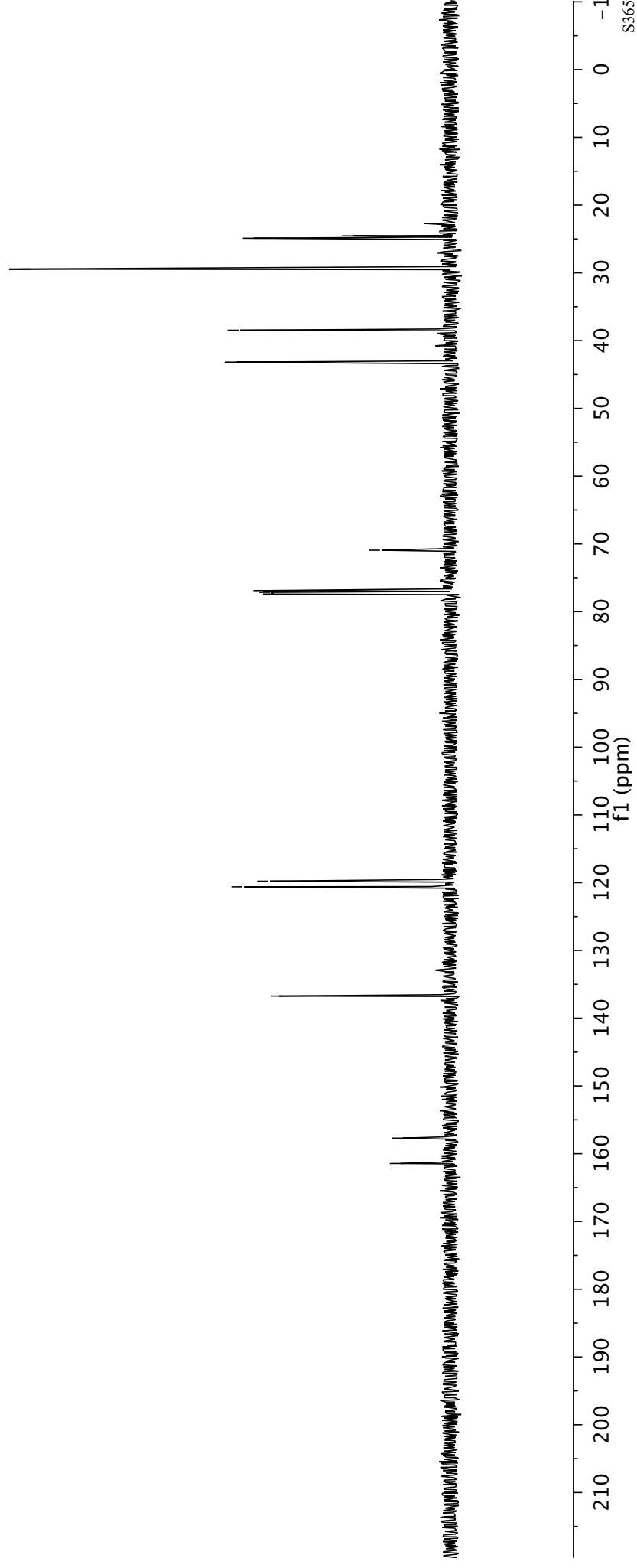
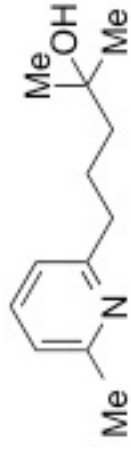
f1 (ppm)

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



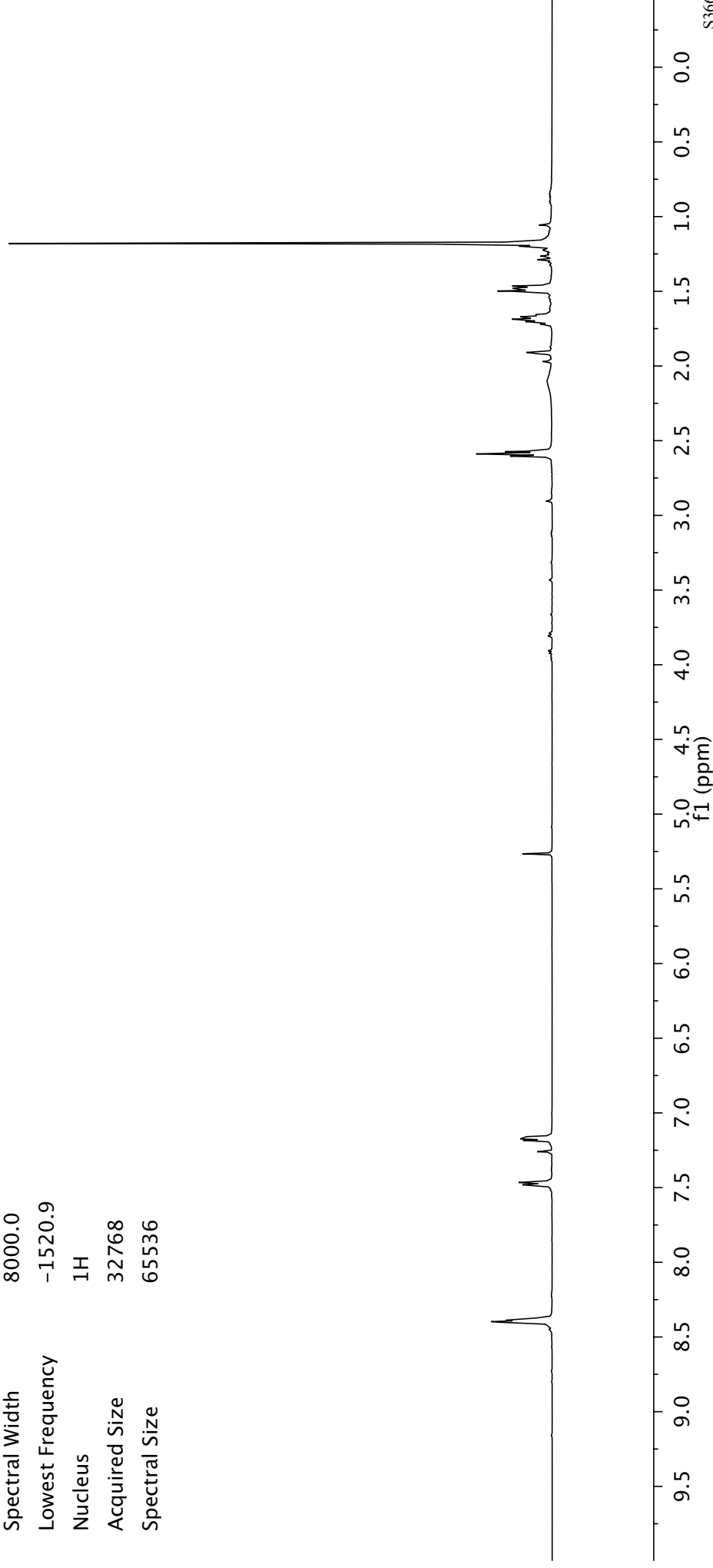
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1276.7
Nucleus	¹³ C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

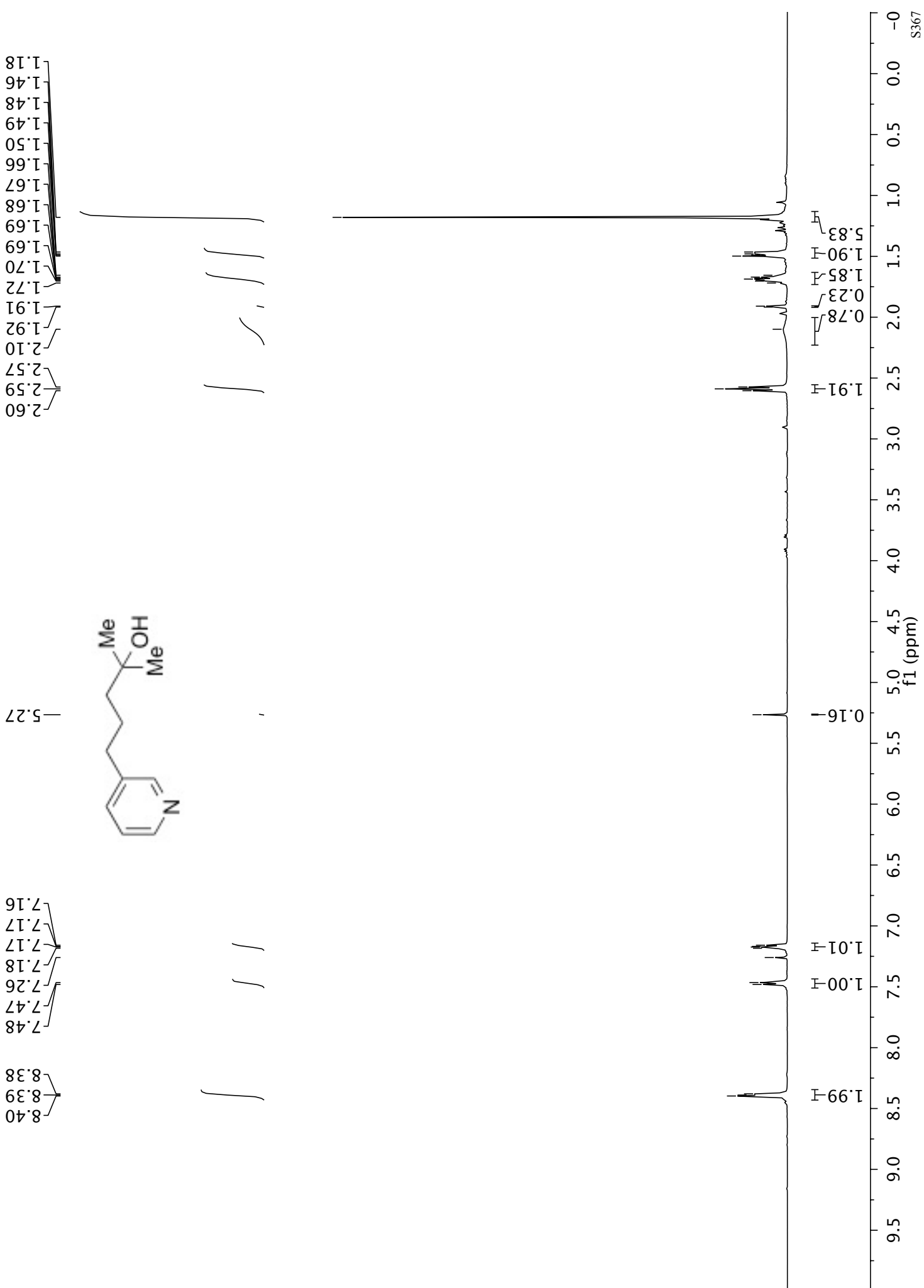






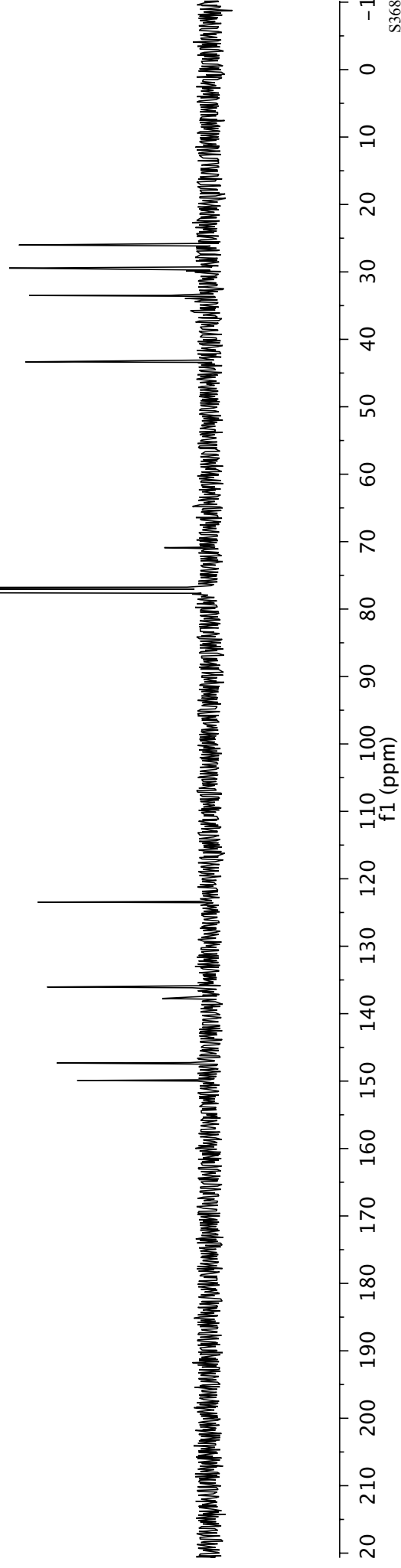
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	22
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1520.9
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

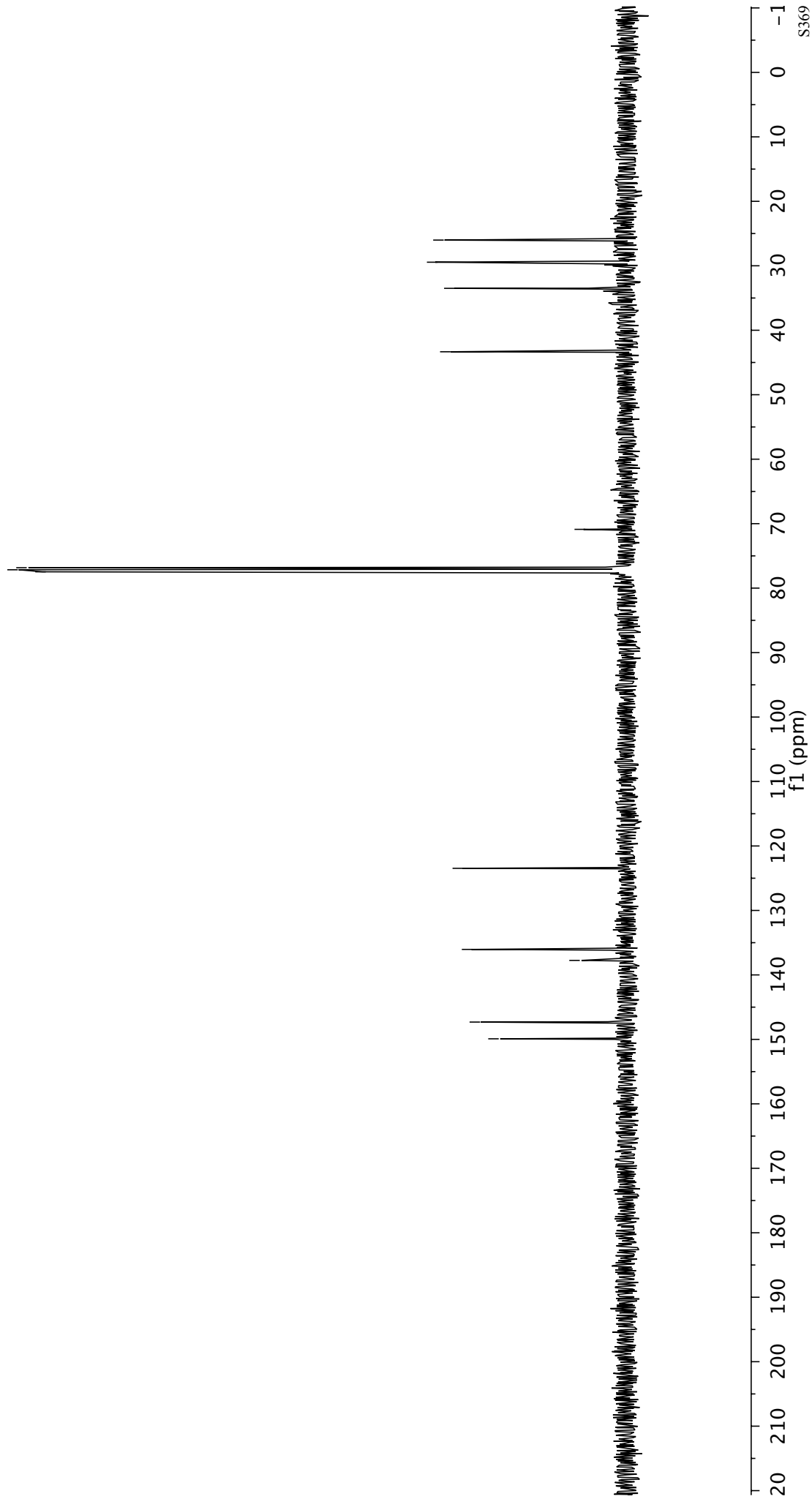
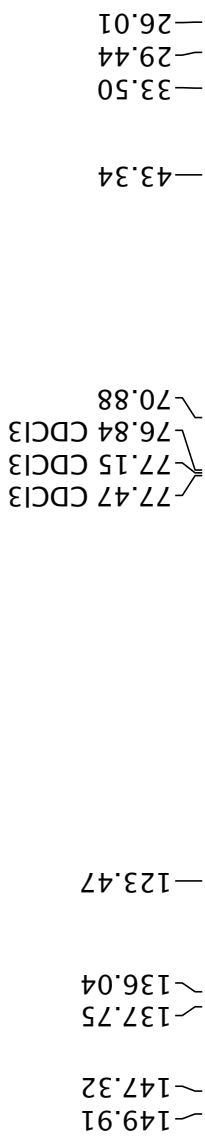


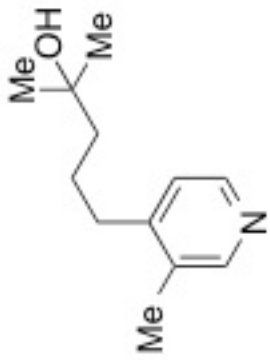




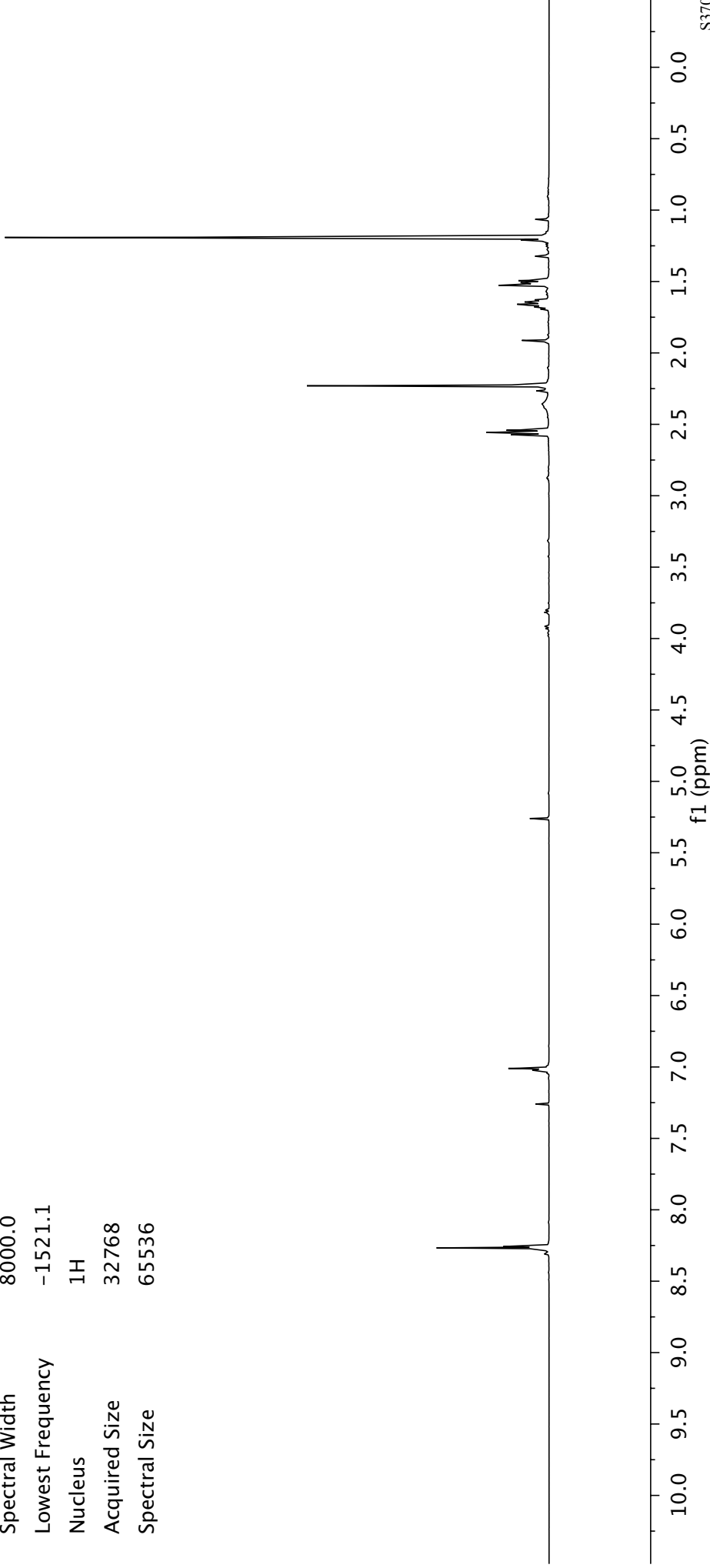
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3107
Spectrometer Frequency	100.58
Spectral Width	25000.0
Lowest Frequency	-1027.1
Nucleus	¹³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

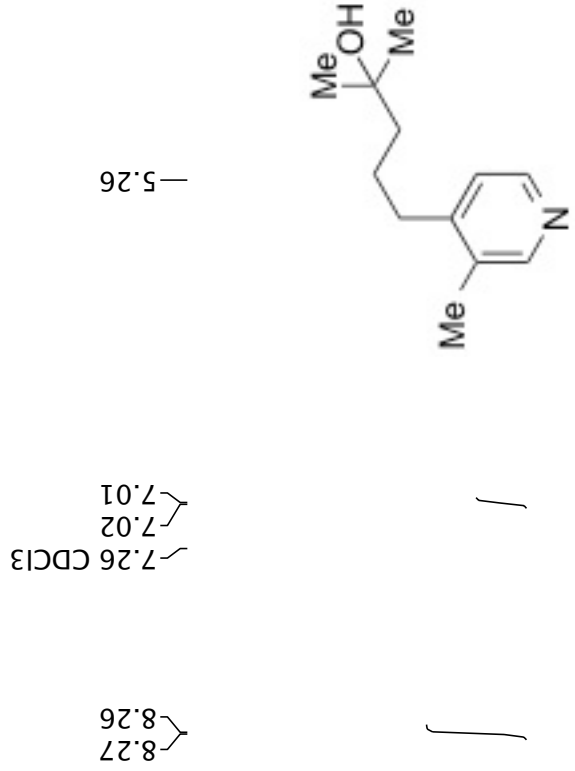






Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	28
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1
Nucleus	¹ H
Acquired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

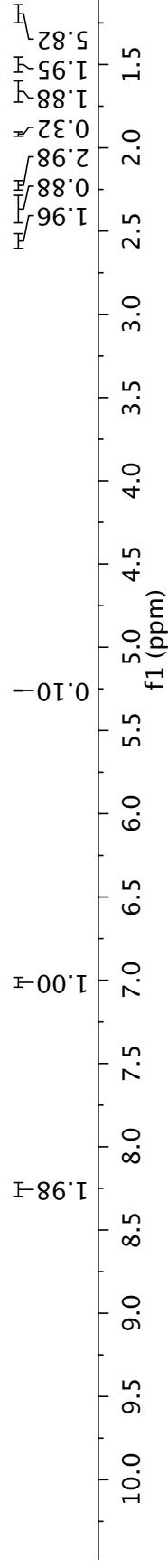


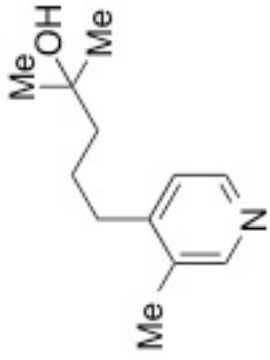


8.27
8.26
7.26 CDCl₃
7.02
7.01

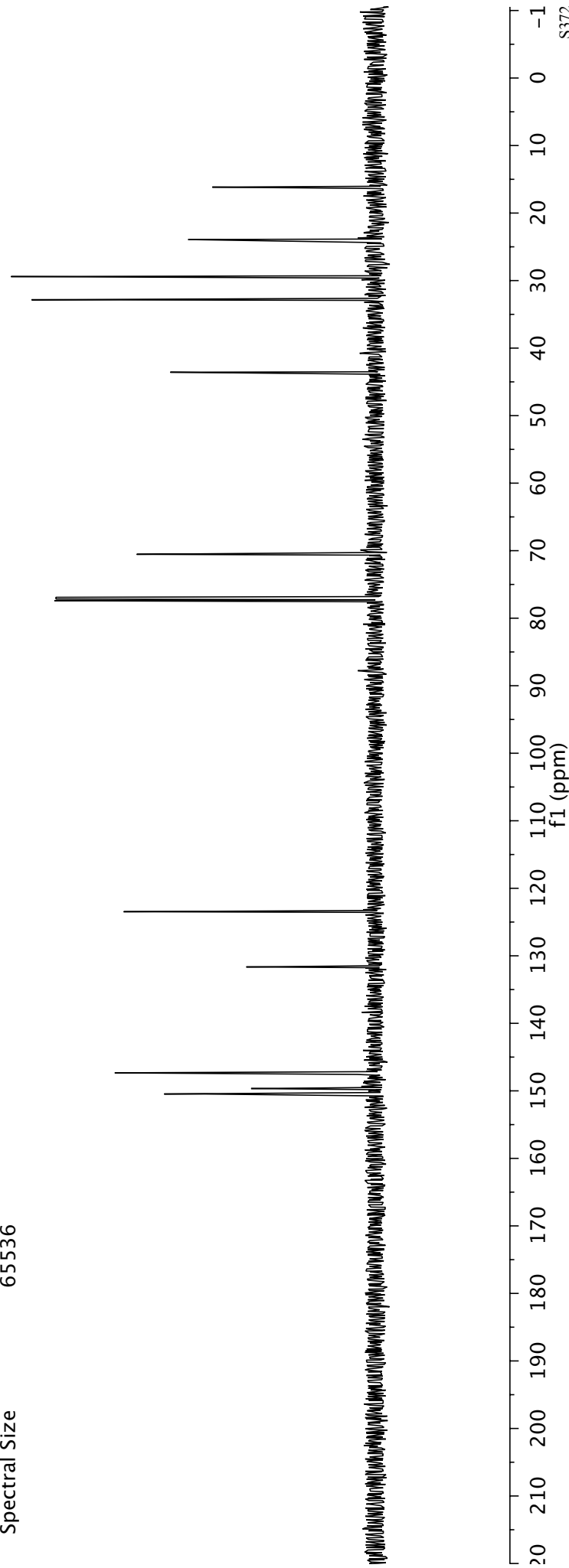
5.26

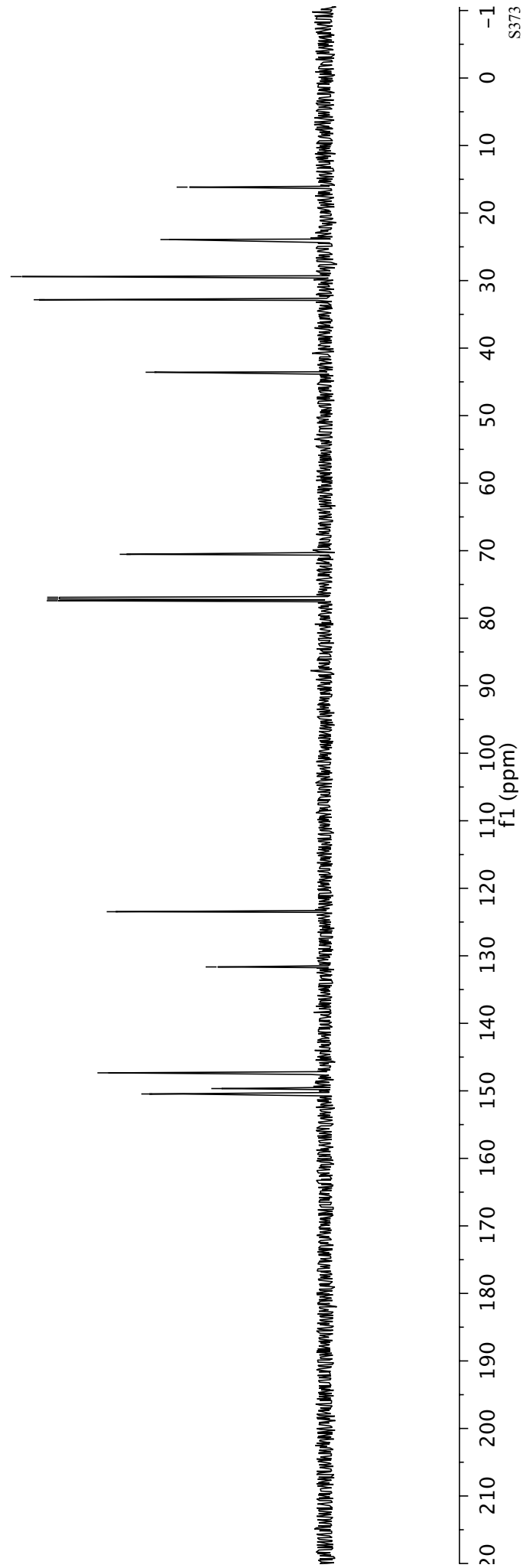
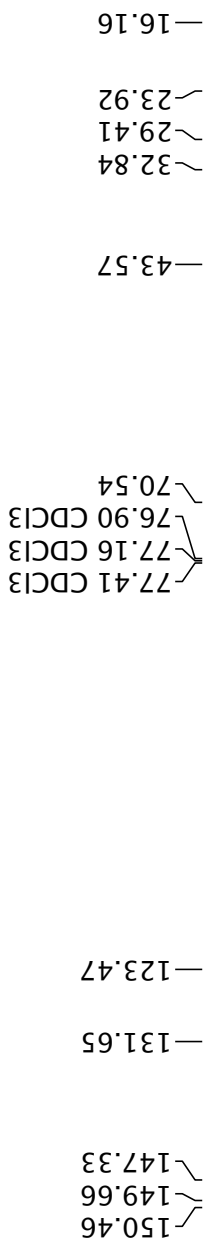
2.57
2.56
2.54
2.36
2.23
2.23
1.91
1.69
1.68
1.68
1.66
1.65
1.64
1.63
1.53
1.52
1.51
1.49
1.19

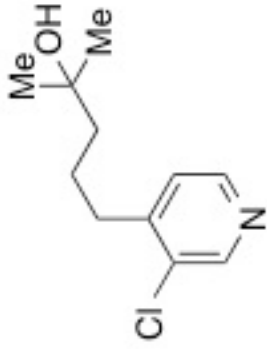




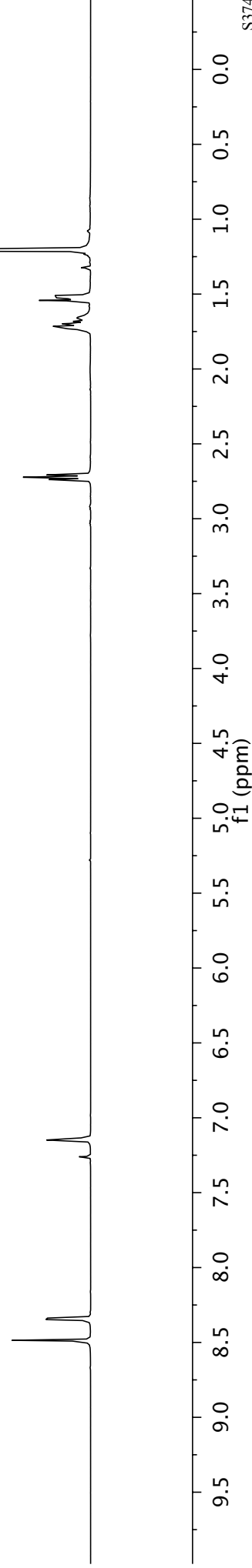
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2208.3
Nucleus	¹³ C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

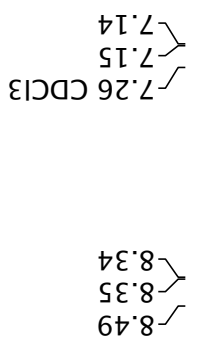
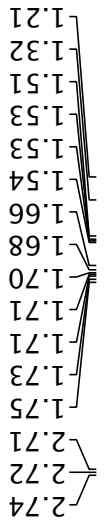
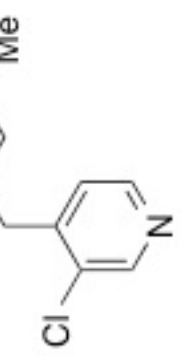
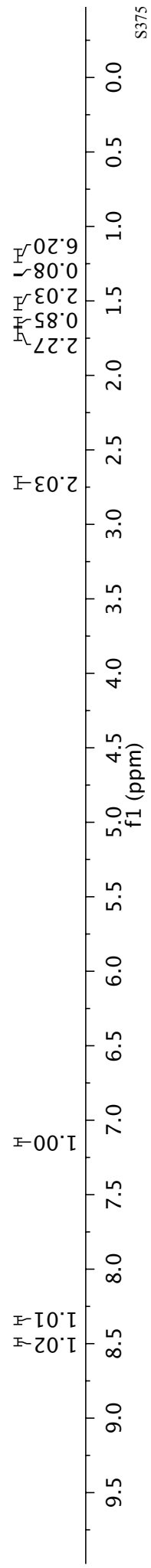


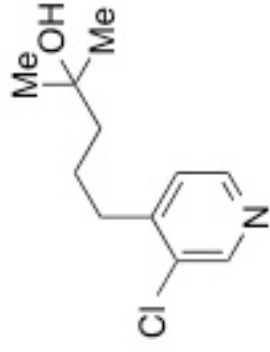




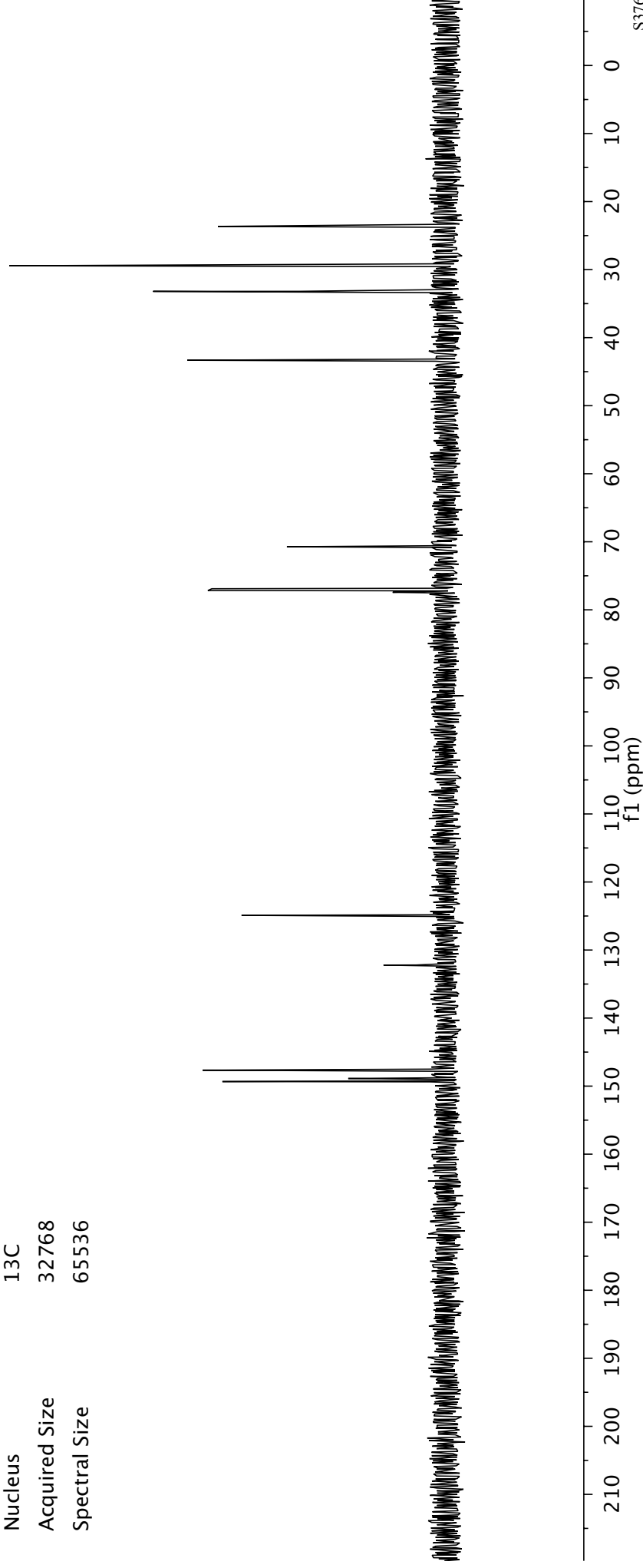
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	26
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1520.6
Nucleus	¹ H
Acquired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

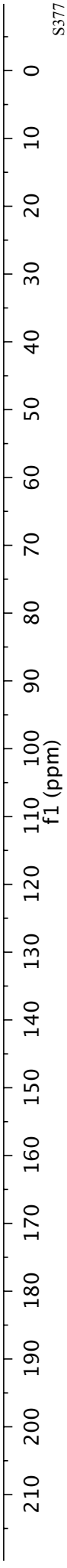
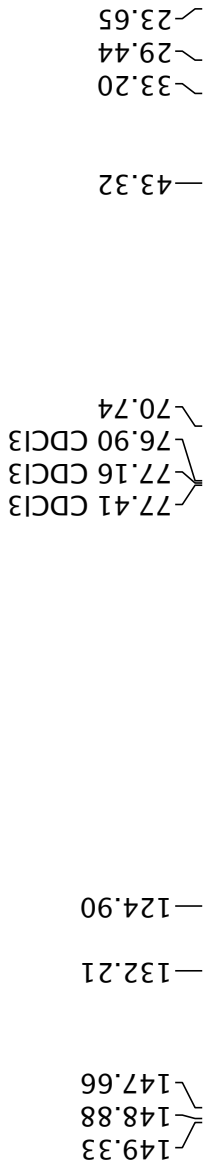
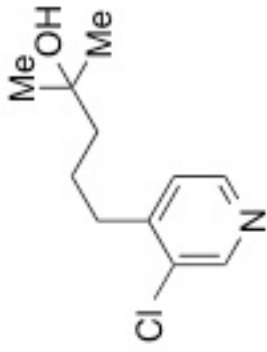




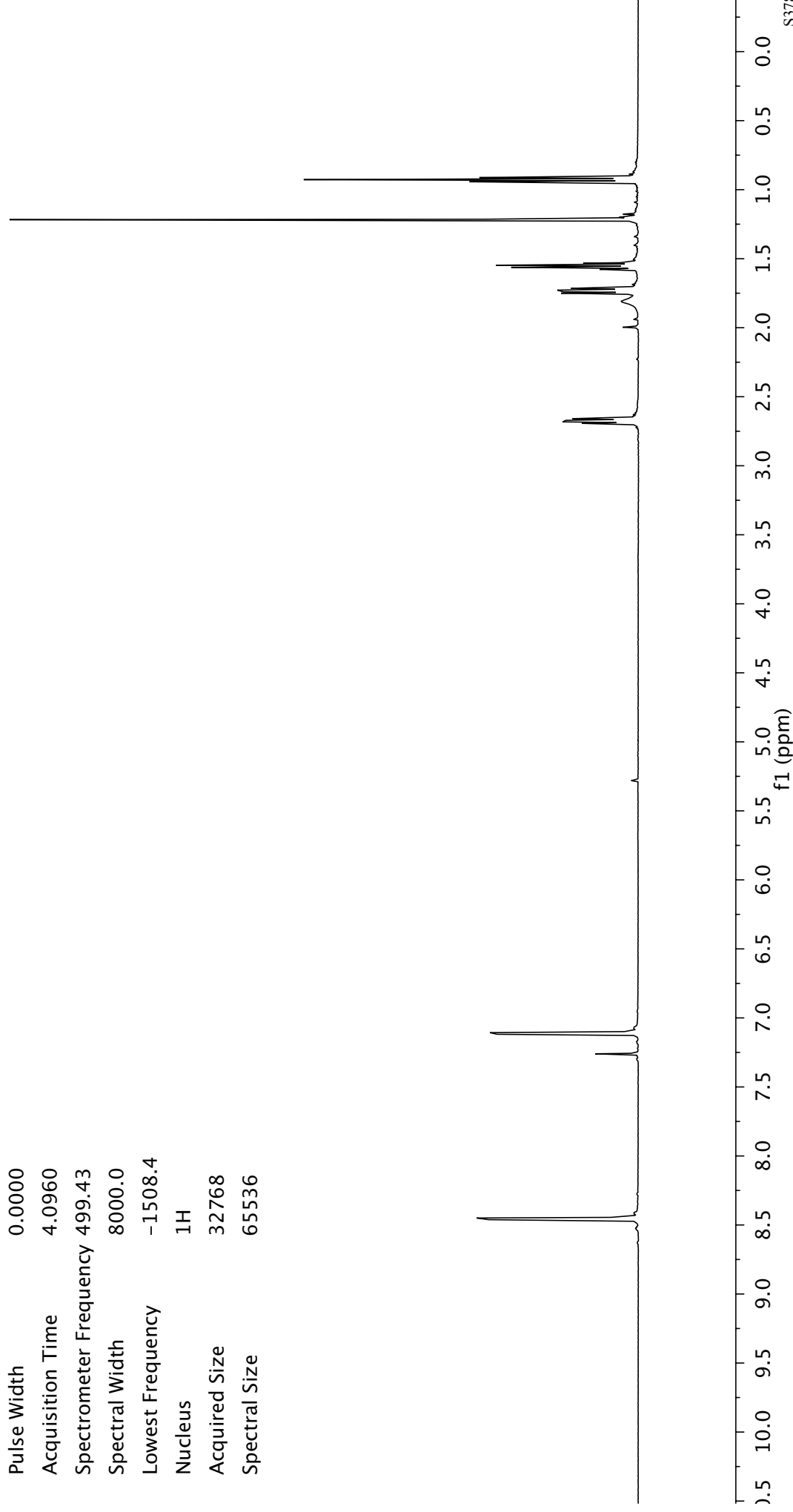
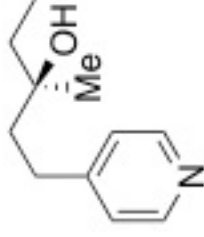


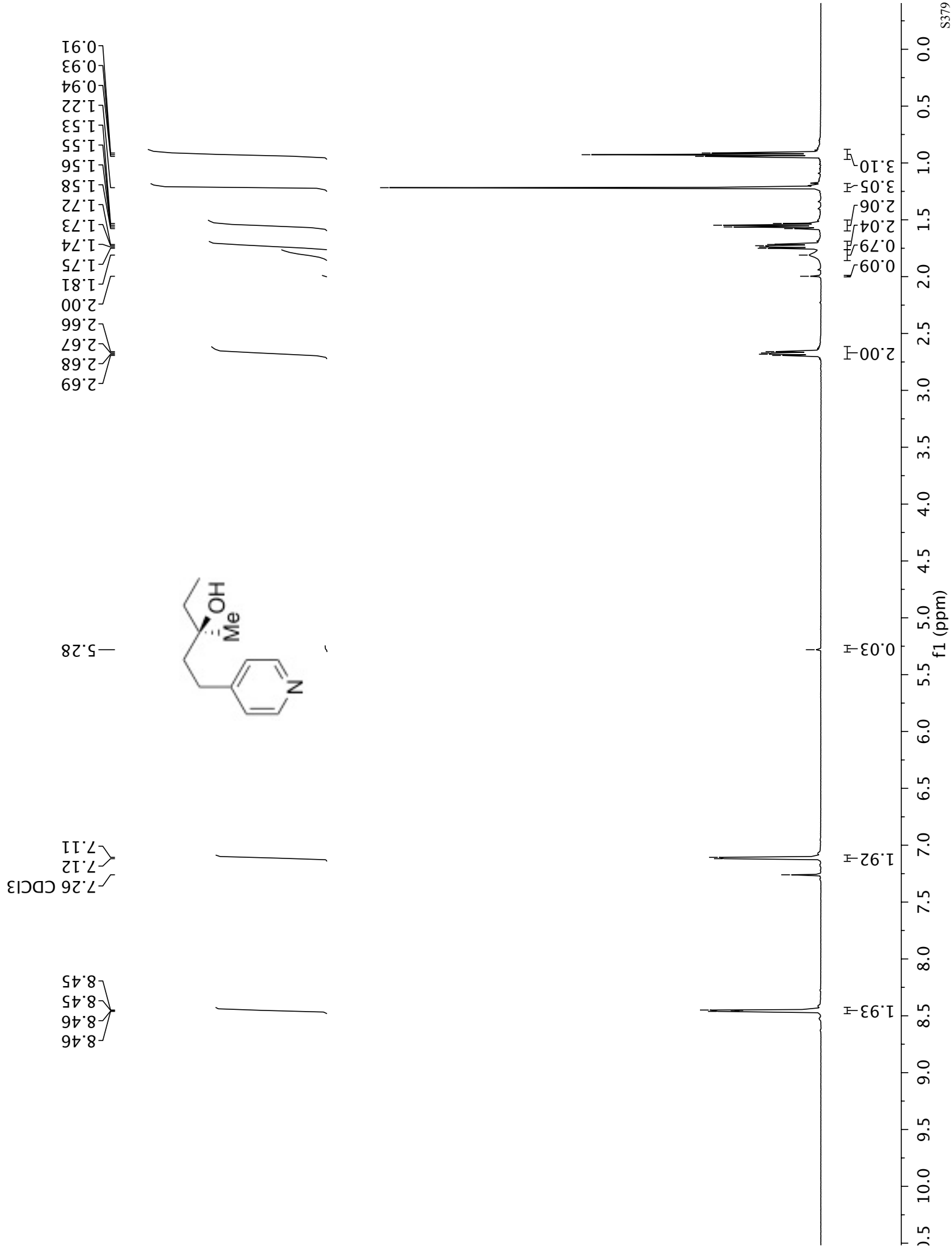
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2205.0
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

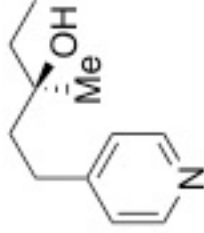




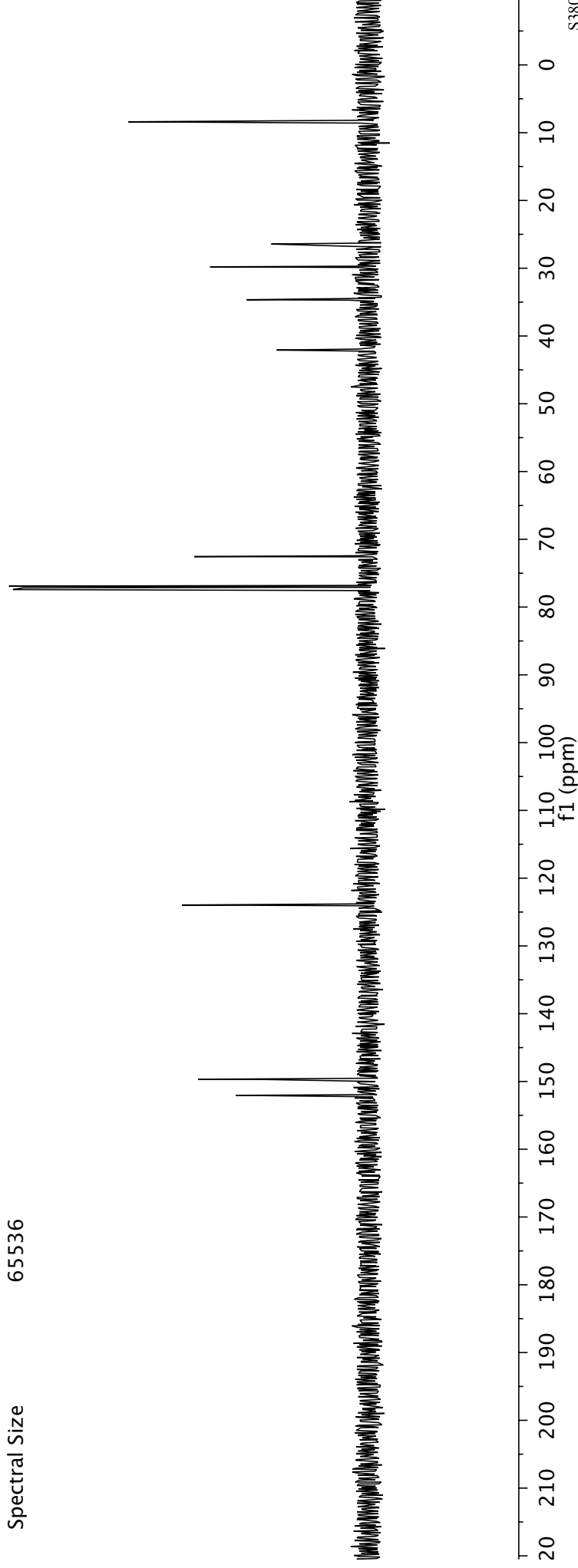
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	56
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	499.43
Spectral Width	8000.0
Lowest Frequency	-1508.4
Nucleus	¹ H
Acquired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

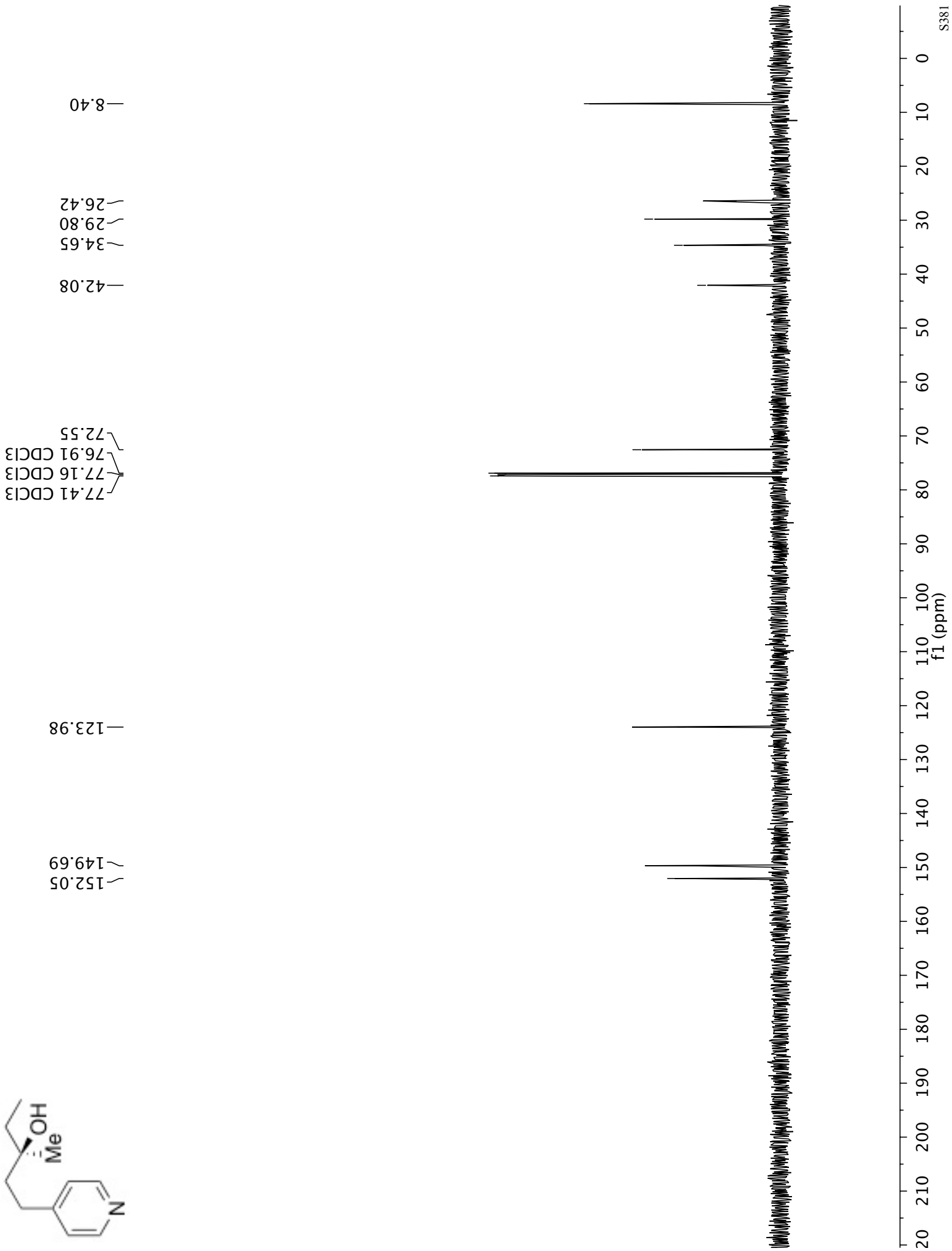
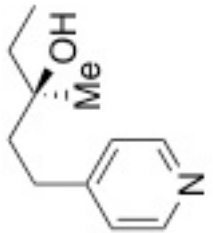


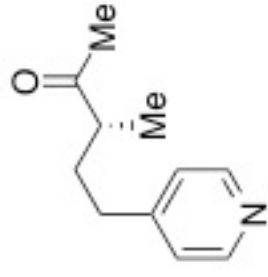




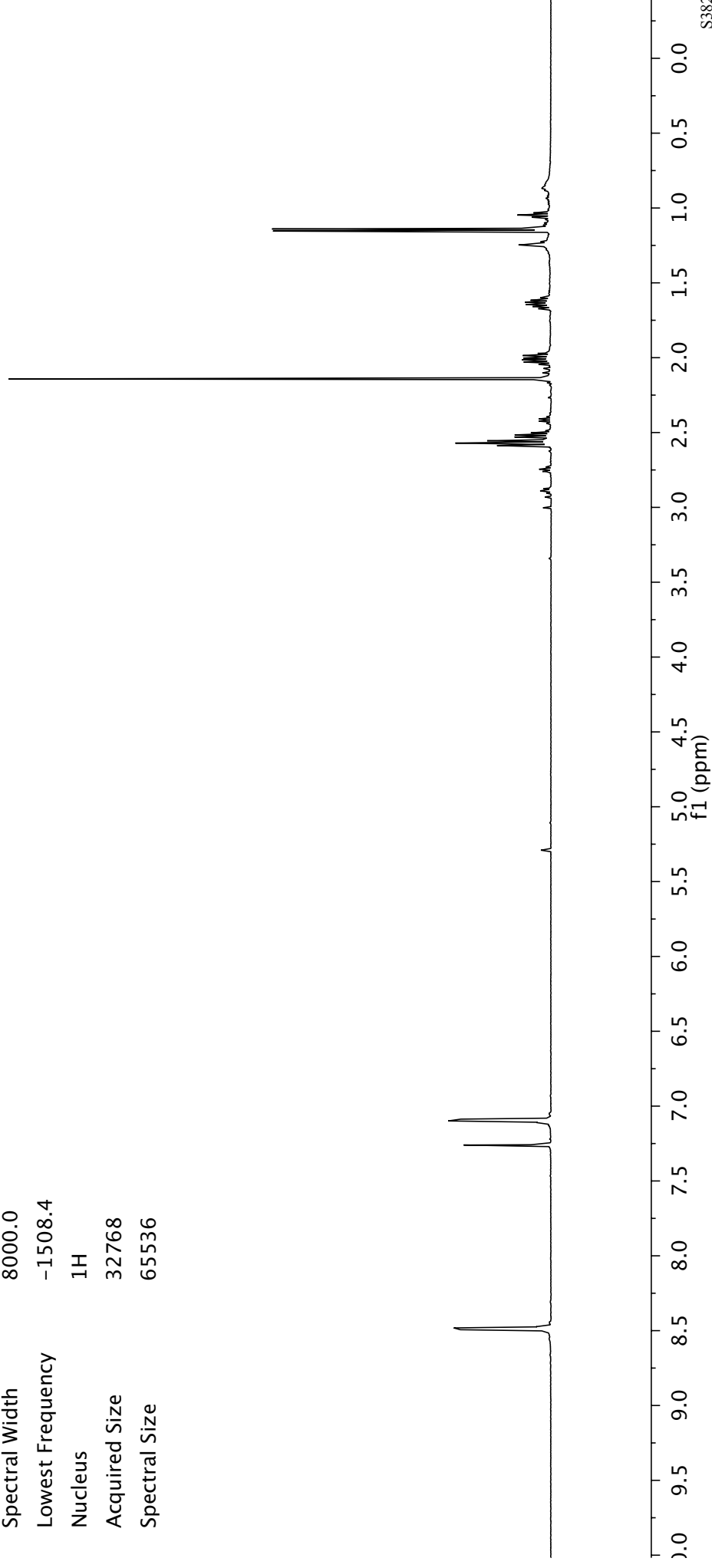
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2202.4
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

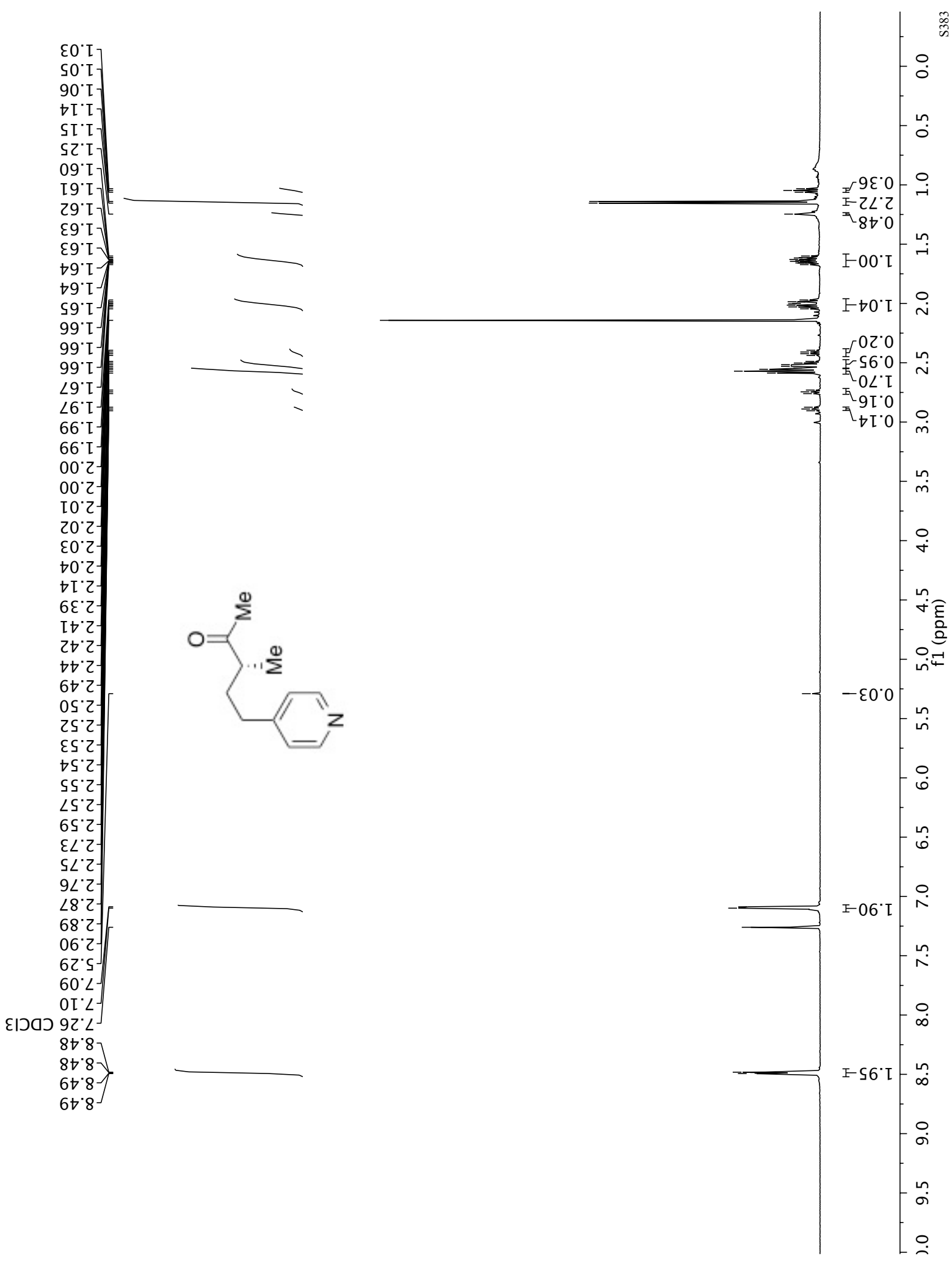


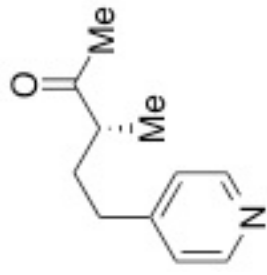




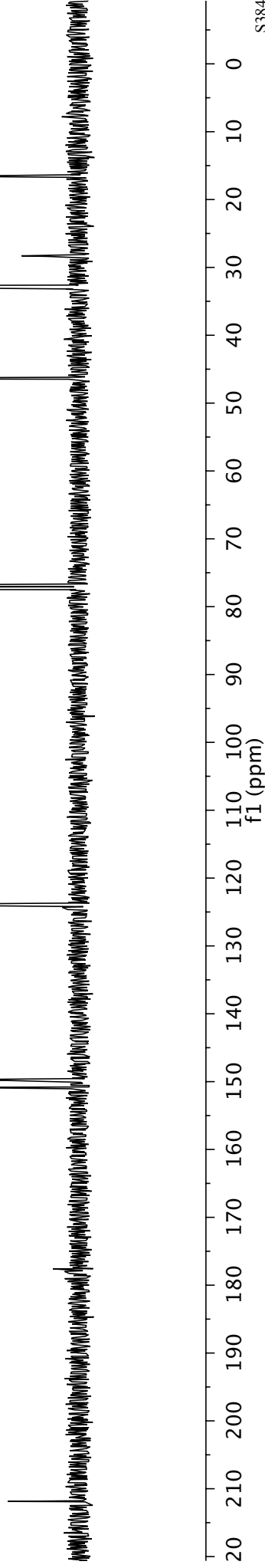
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	56
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	499.43
Spectral Width	8000.0
Lowest Frequency	-1508.4
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

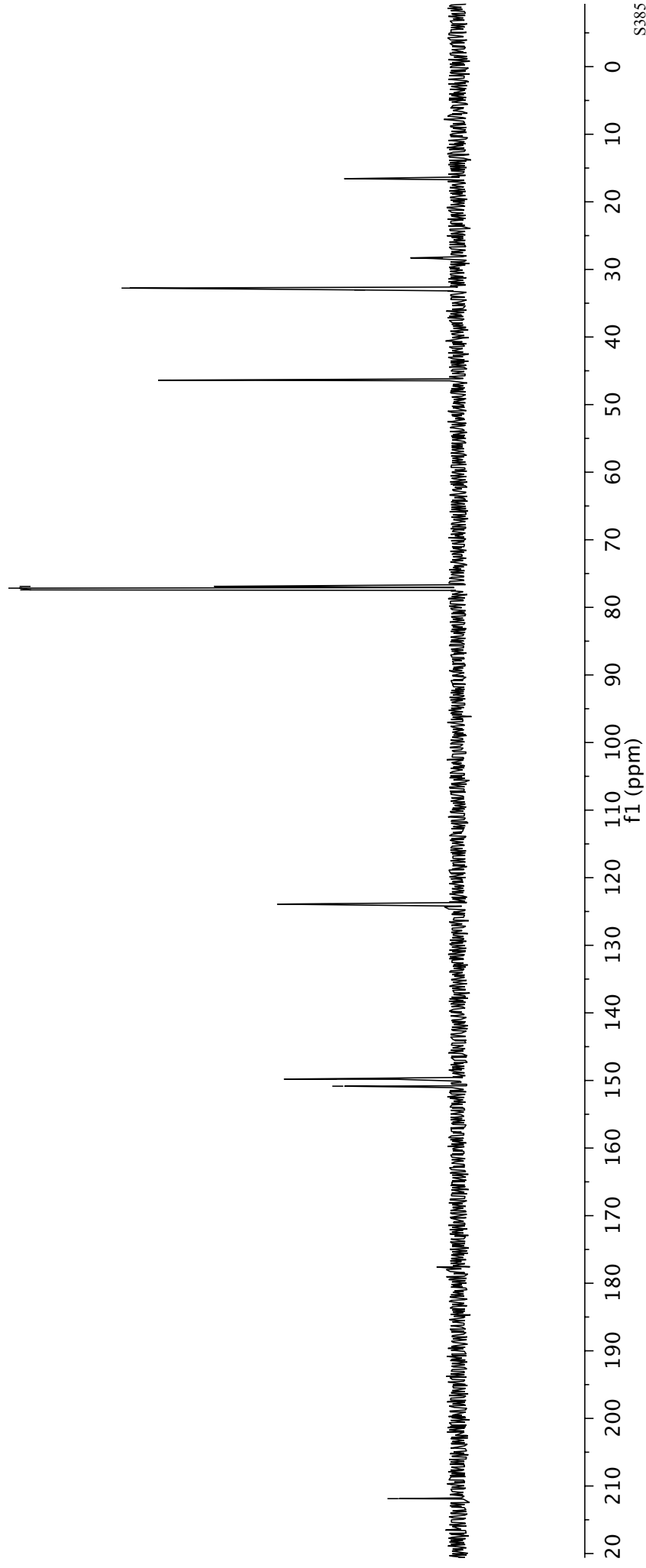
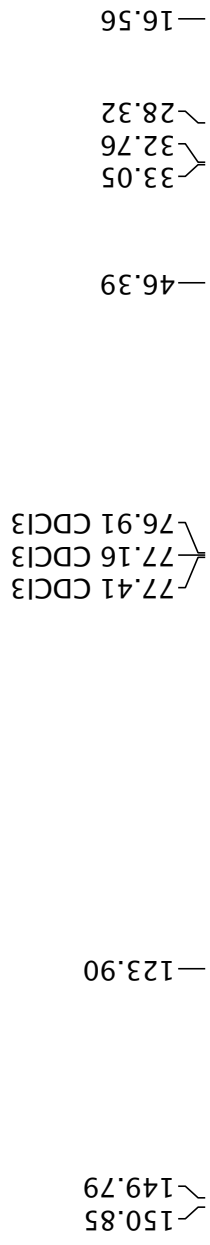
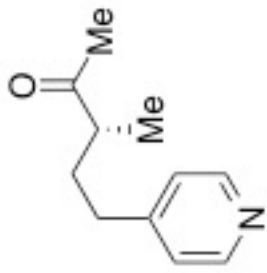


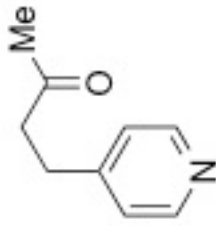




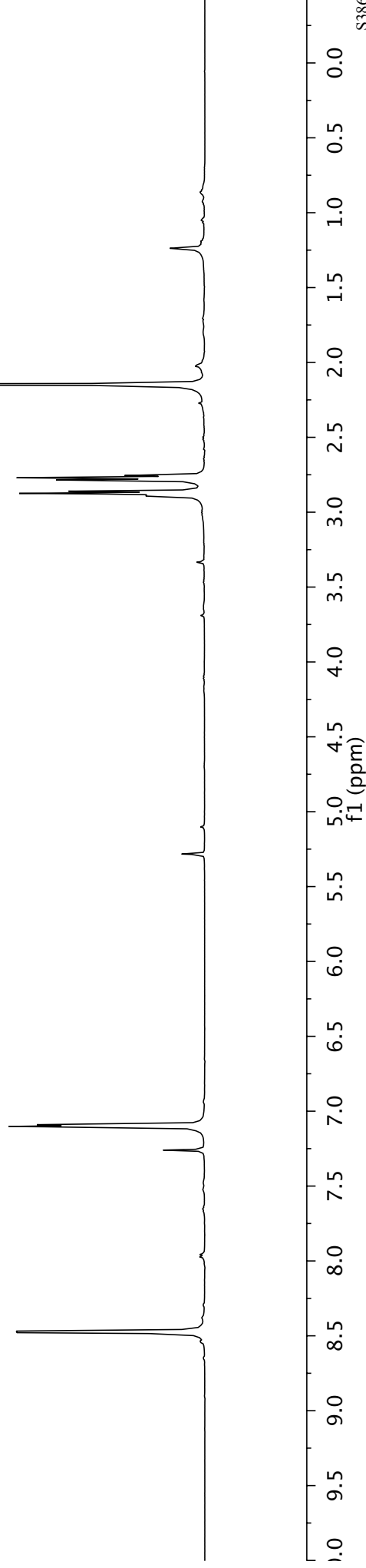
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2207.0
Nucleus	¹³ C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

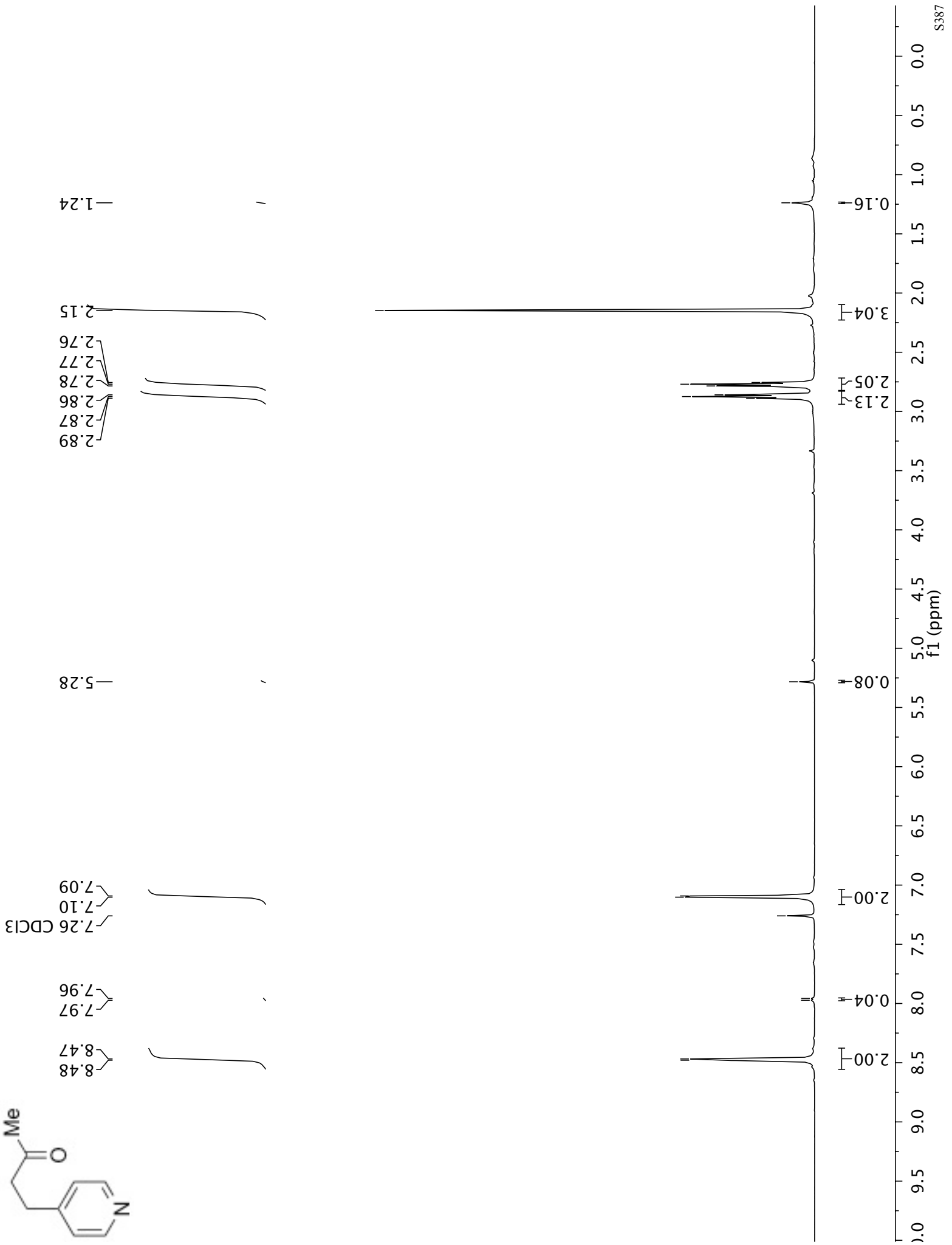
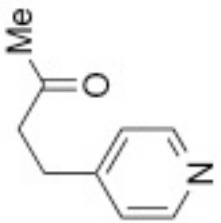


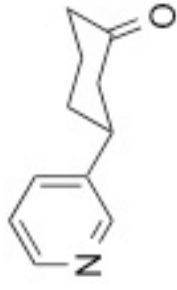




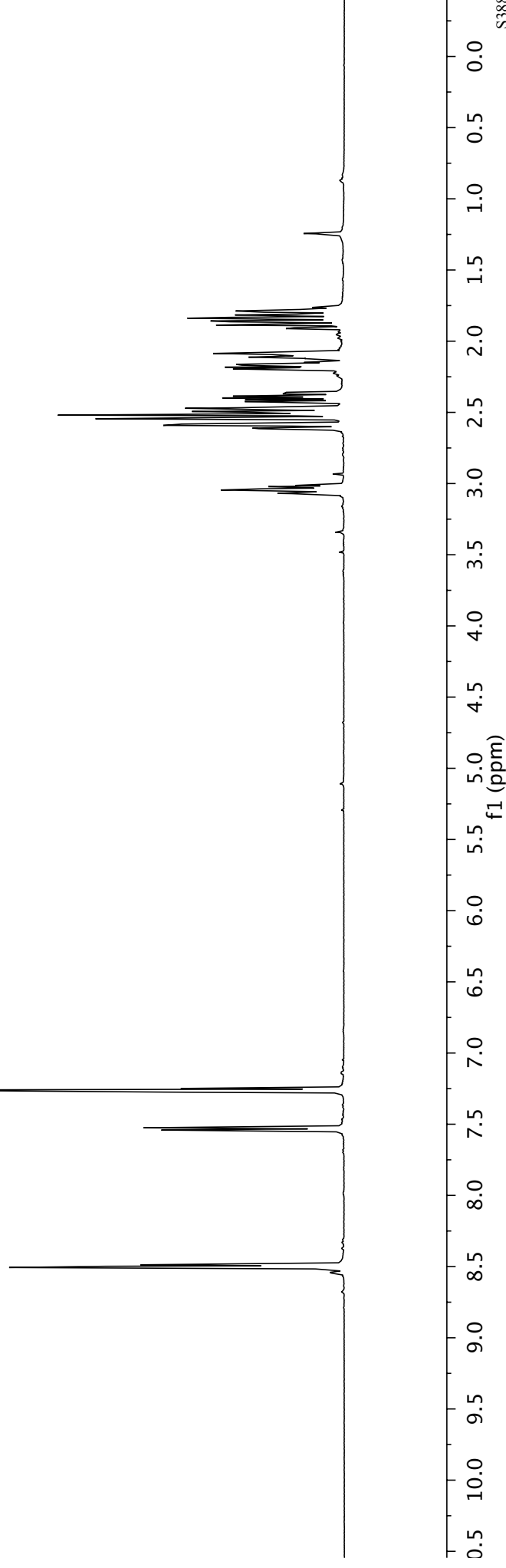
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	32
Relaxation Delay	10.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1520.9
Nucleus	¹ H
Acquired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

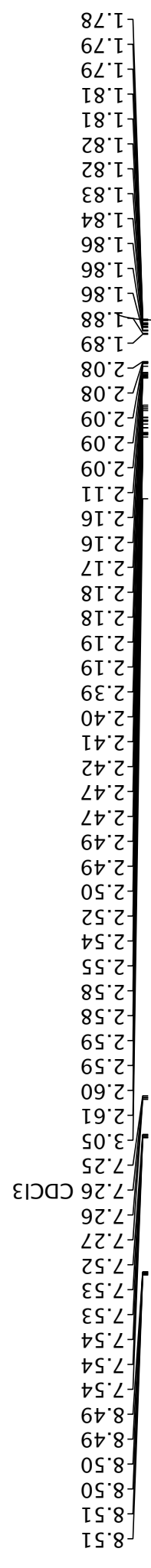
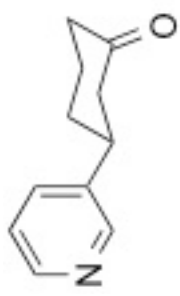
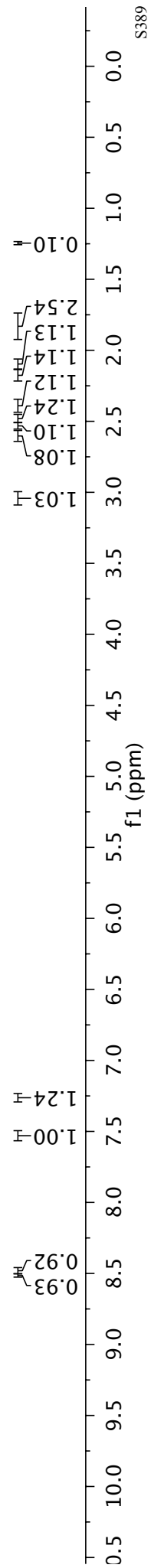






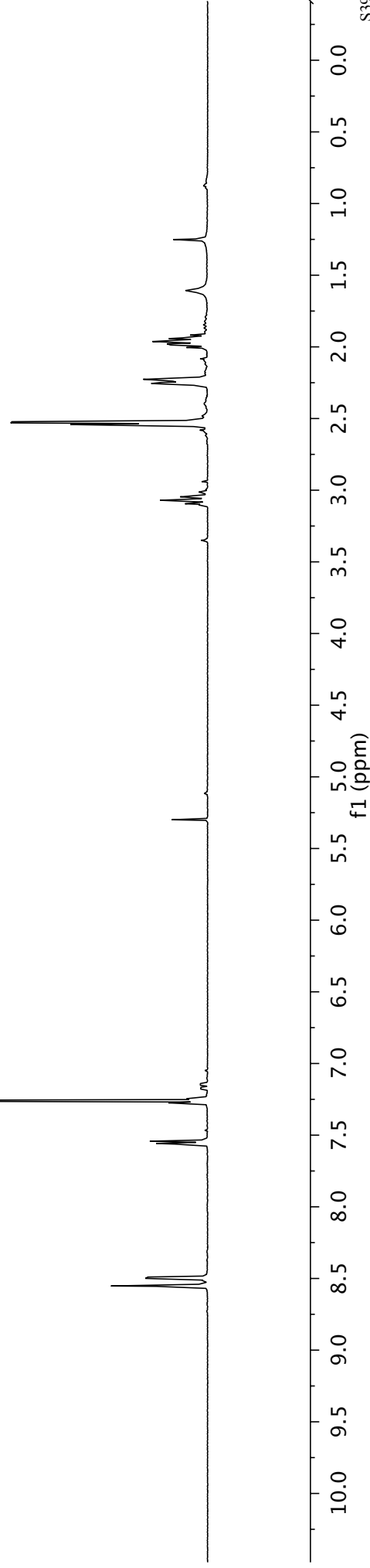
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	48
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1520.9
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

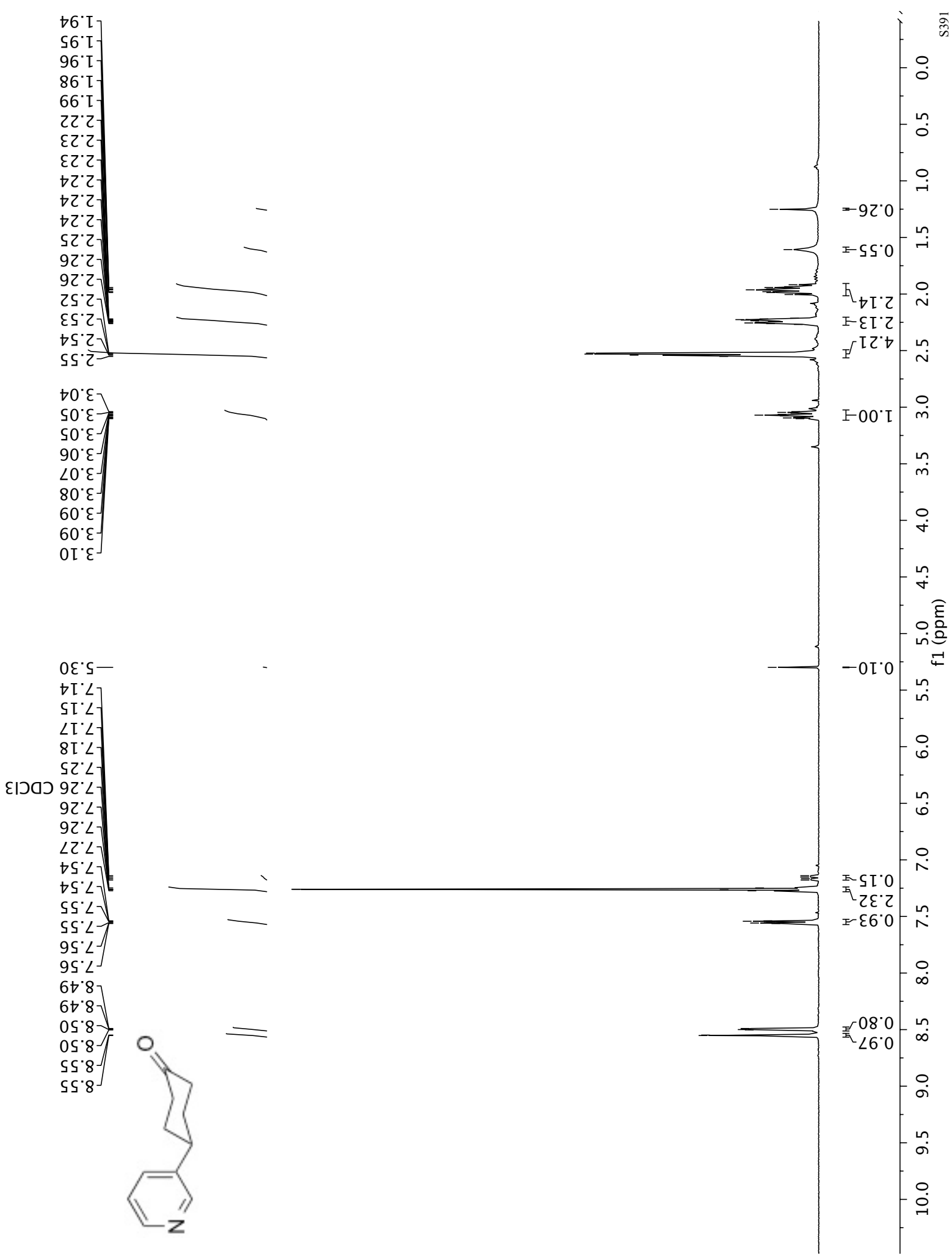




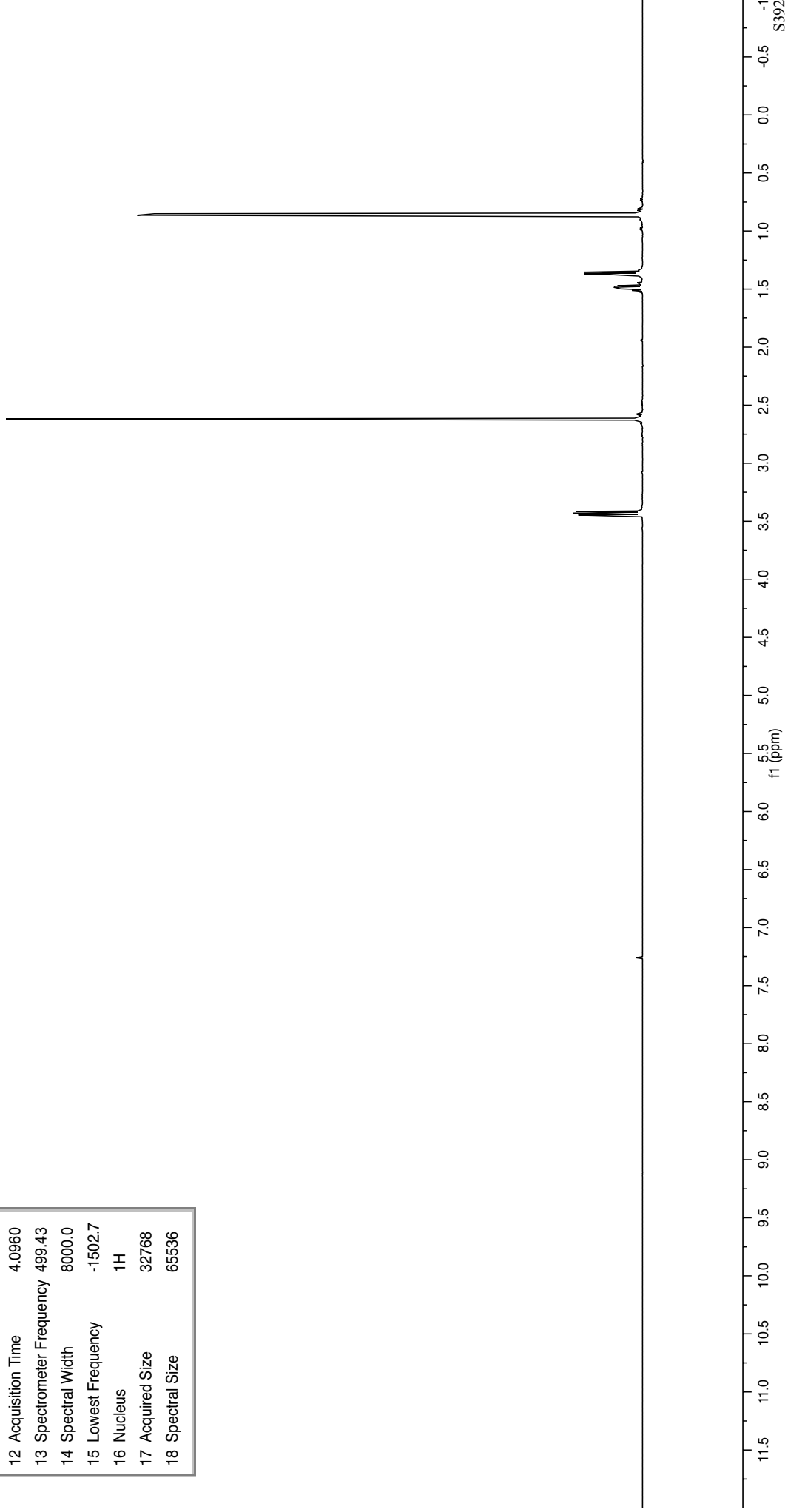
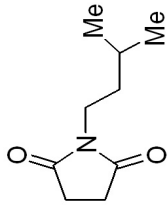


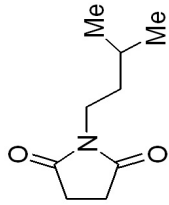
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1520.6
Nucleus	¹ H
Acquired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



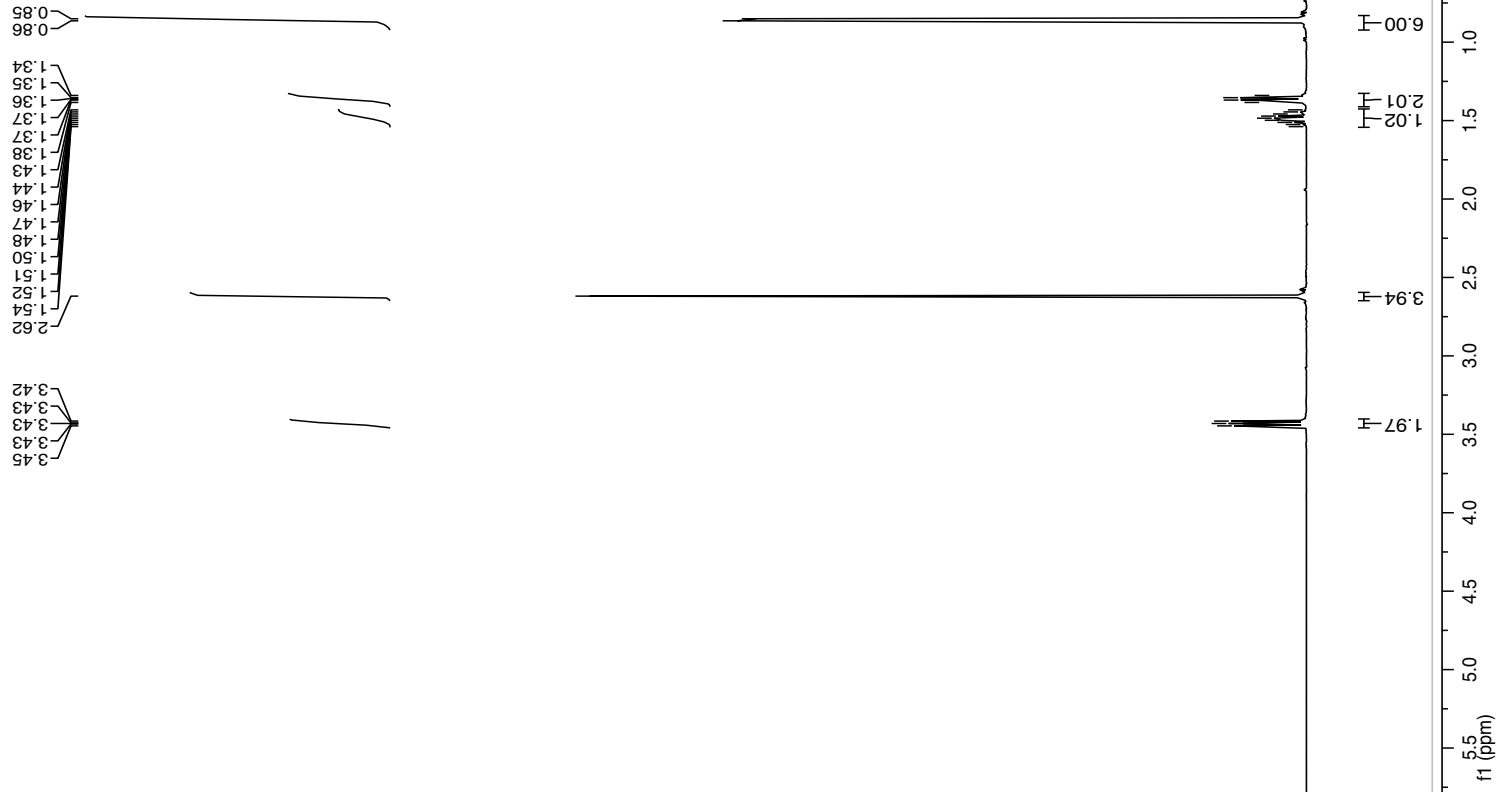


Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUADG
8 Number of Scans	8
9 Receiver Gain	44
10 Relaxation Delay	0.0000
11 Pulse Width	0.0000
12 Acquisition Time	4.0960
13 Spectrometer Frequency	499.43
14 Spectral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

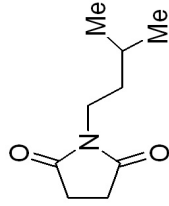




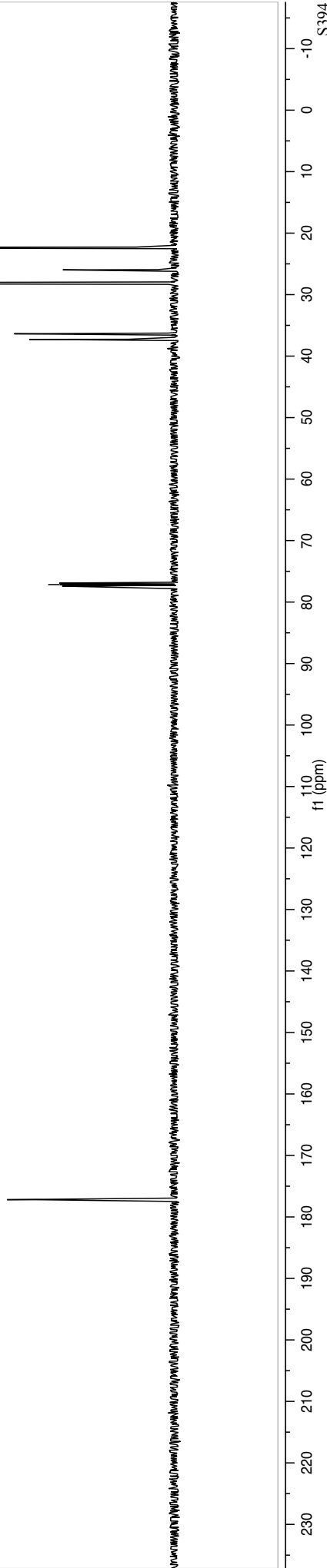
7.26 CDCl₃

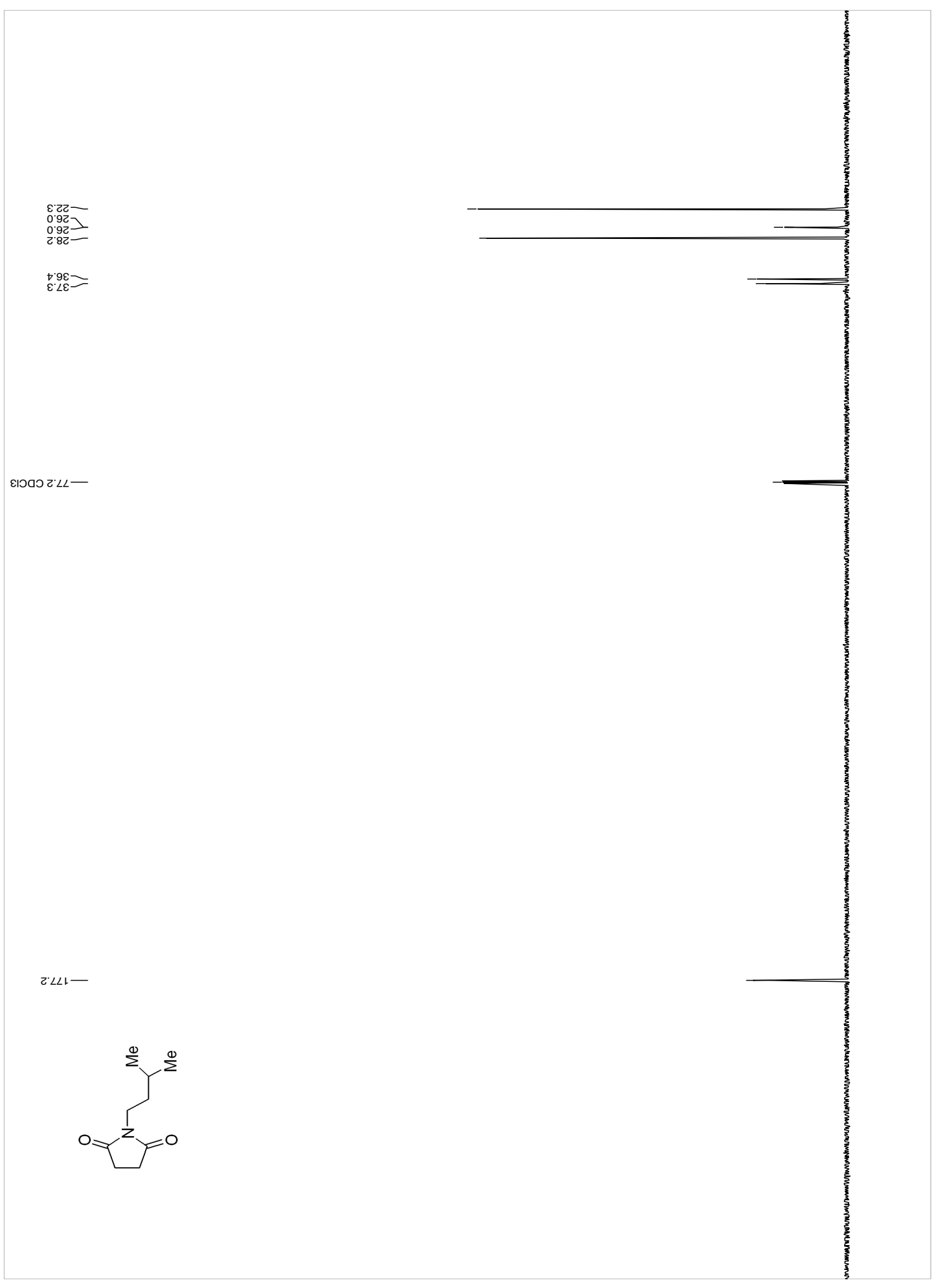


— 77.16 CDCl₃



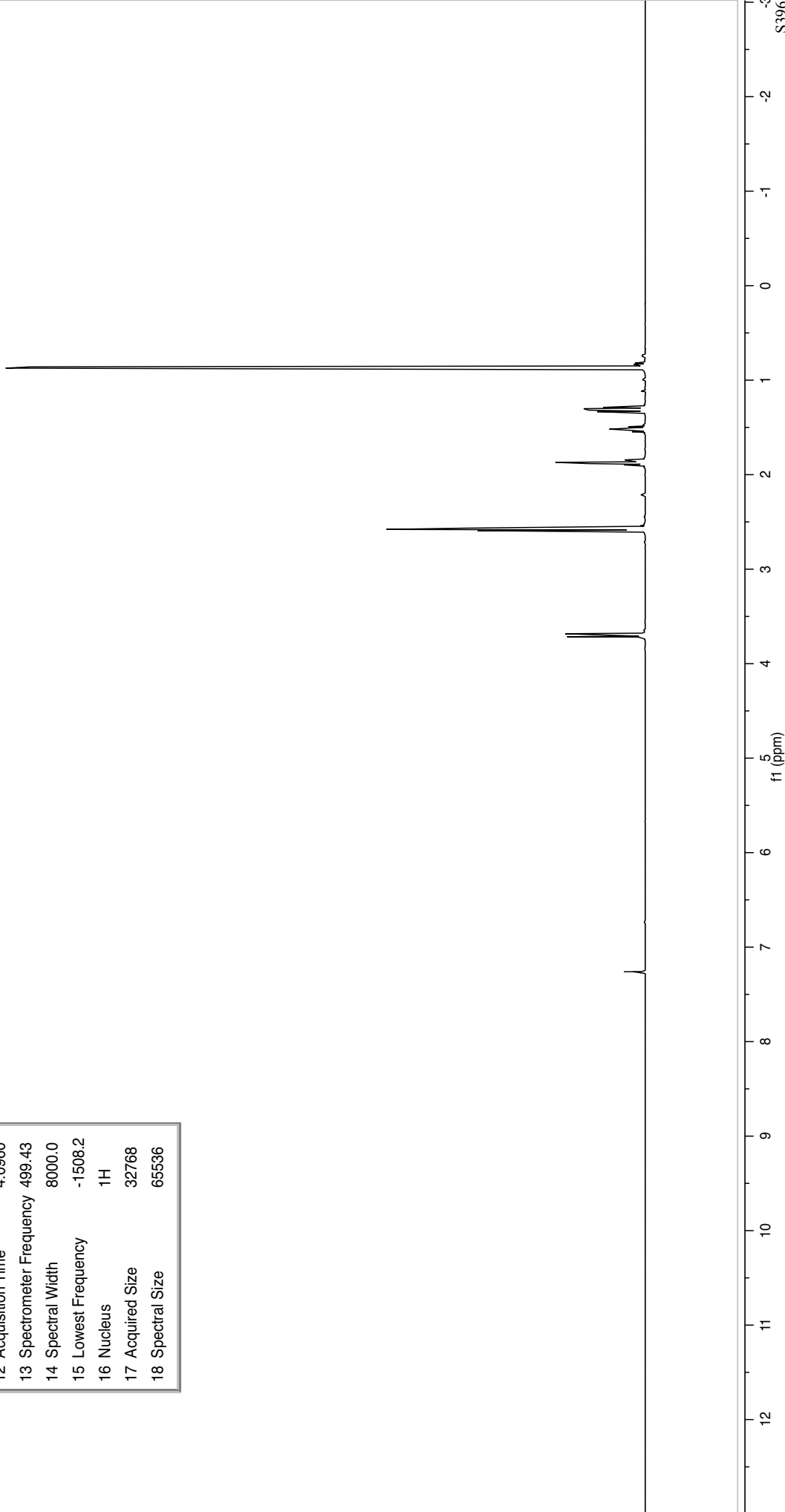
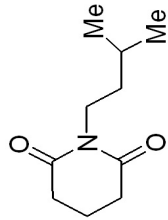
Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl ₃
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUADG
8 Number of Scans	48
9 Receiver Gain	60
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.0240
13 Spectrometer Frequency	125.60
14 Spectral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

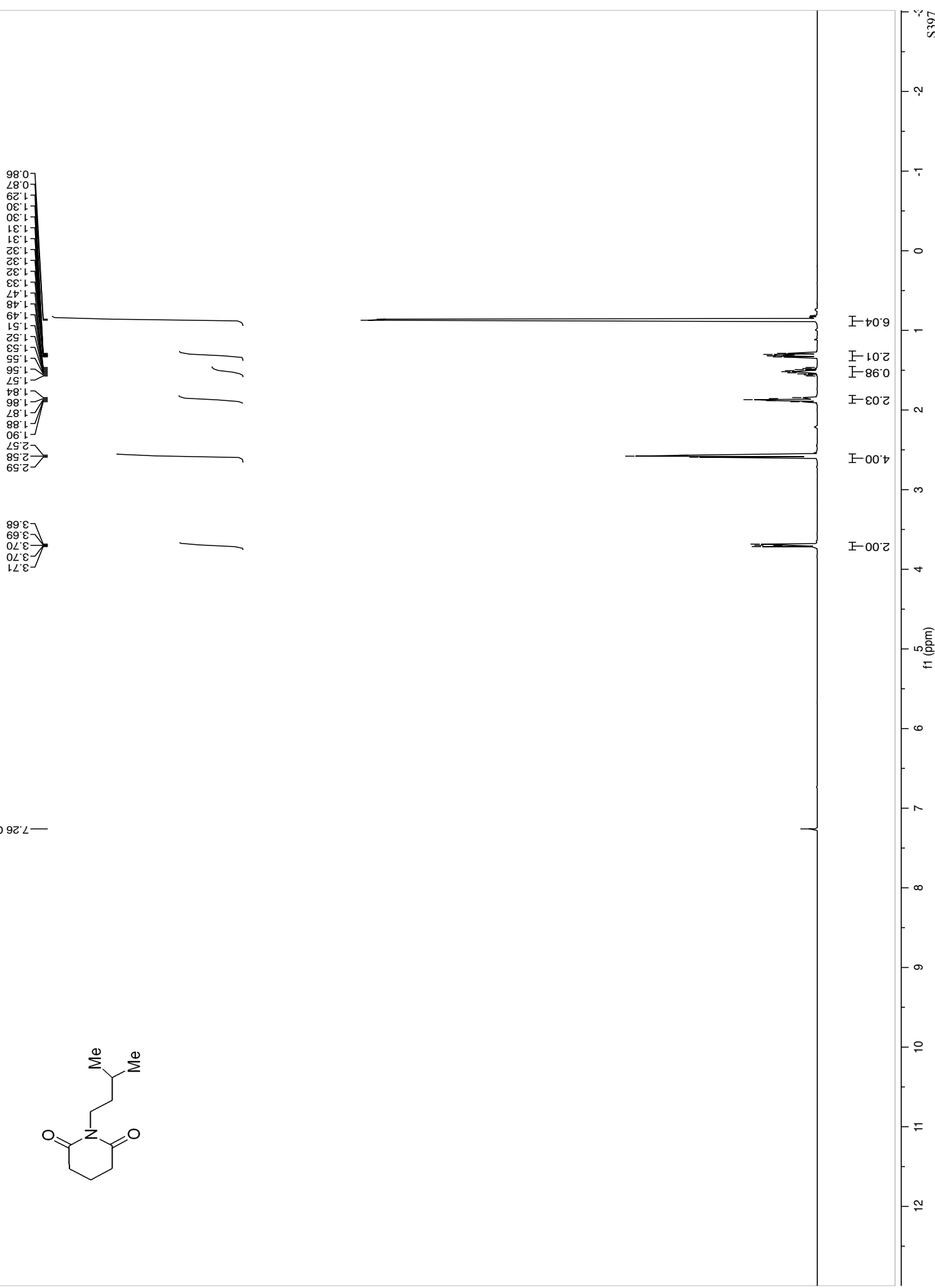




7.26 CDCl3

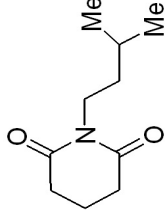
Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUADG
8 Number of Scans	8
9 Receiver Gain	44
10 Relaxation Delay	0.0000
11 Pulse Width	0.0000
12 Acquisition Time	4.0960
13 Spectrometer Frequency	499.43
14 Spectral Width	8000.0
15 Lowest Frequency	-1508.2
16 Nucleus	1H
17 Acquired Size	32768
18 Spectral Size	65536



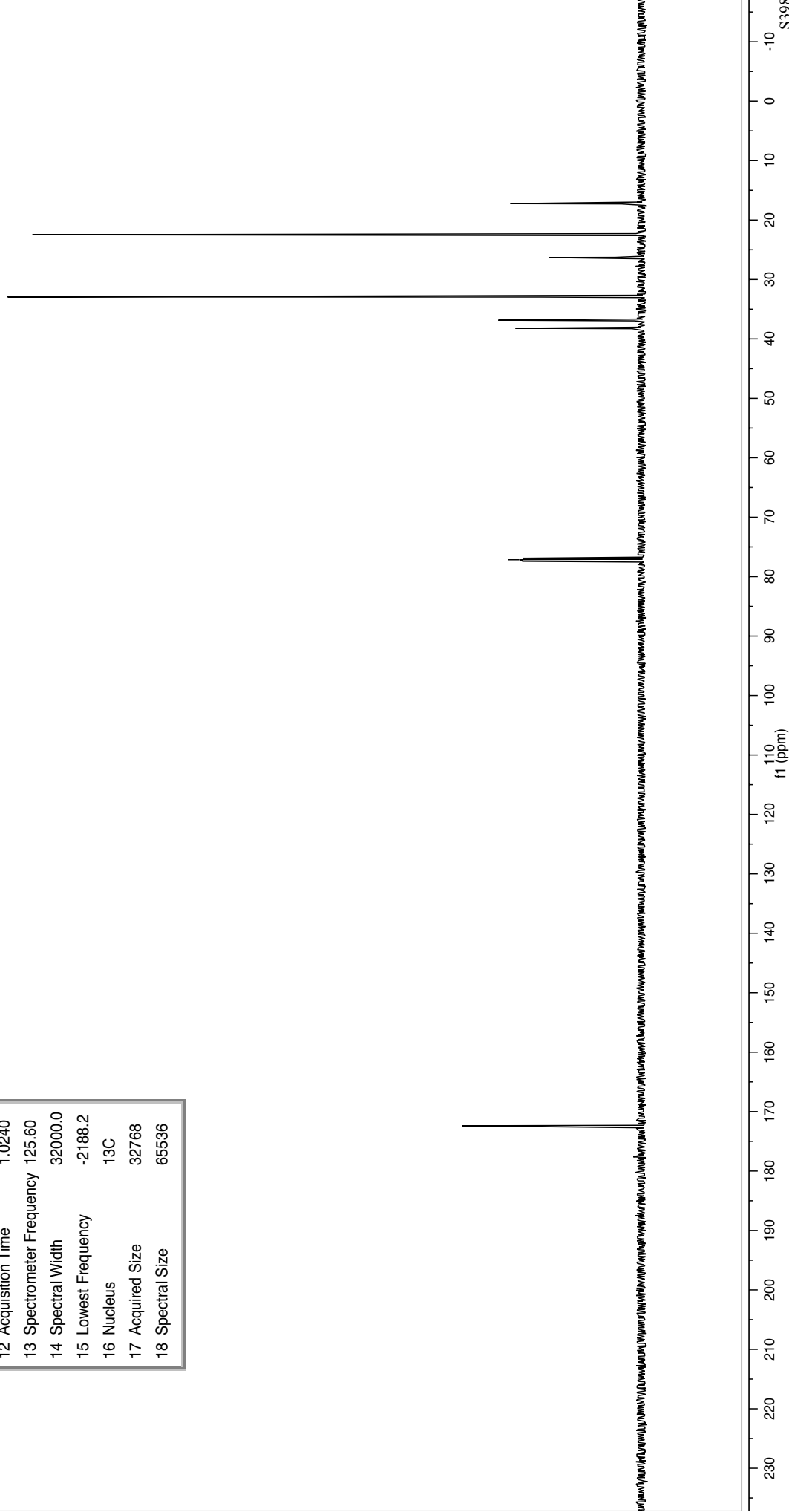


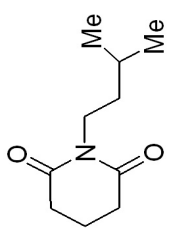
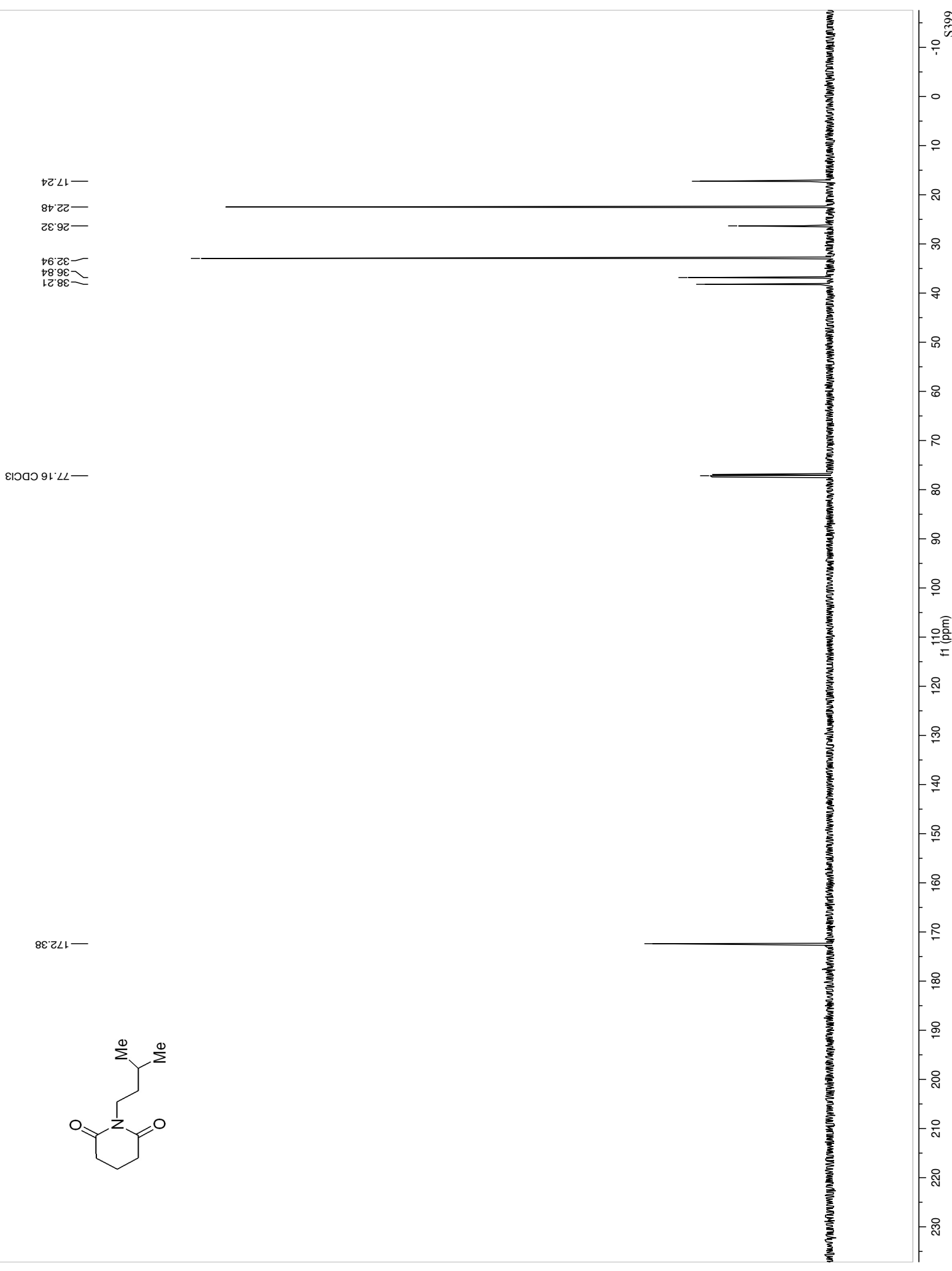
7.26 CDCl₃

Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	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	¹³ C
17 Acquired Size	32768
18 Spectral Size	65536



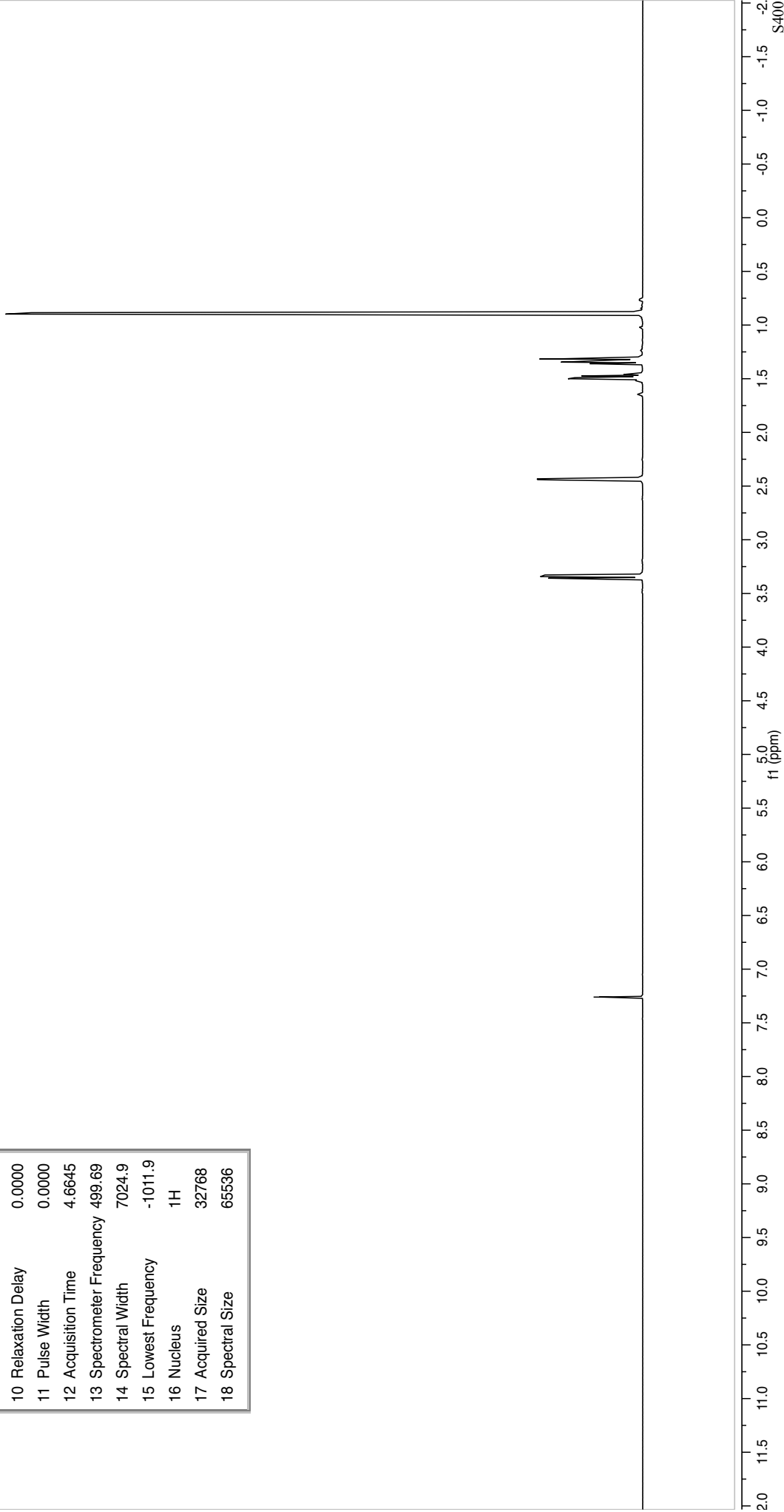
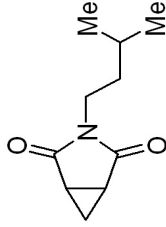
— 77.16 CDCl3

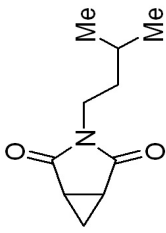




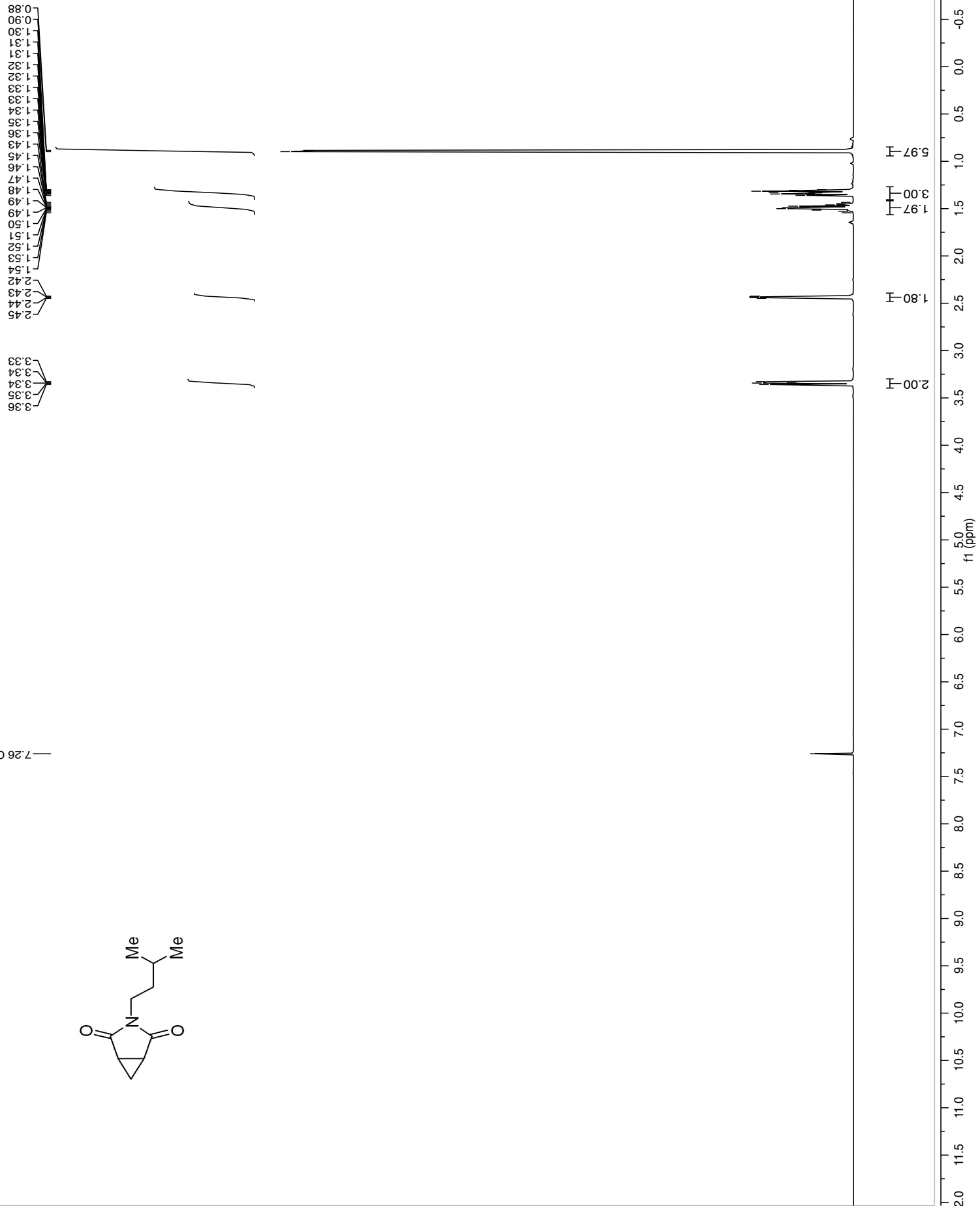
7.26 CDCl3

Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	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	-1011.9
16 Nucleus	1H
17 Acquired Size	32768
18 Spectral Size	65536

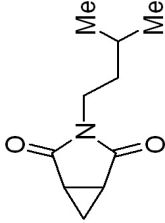




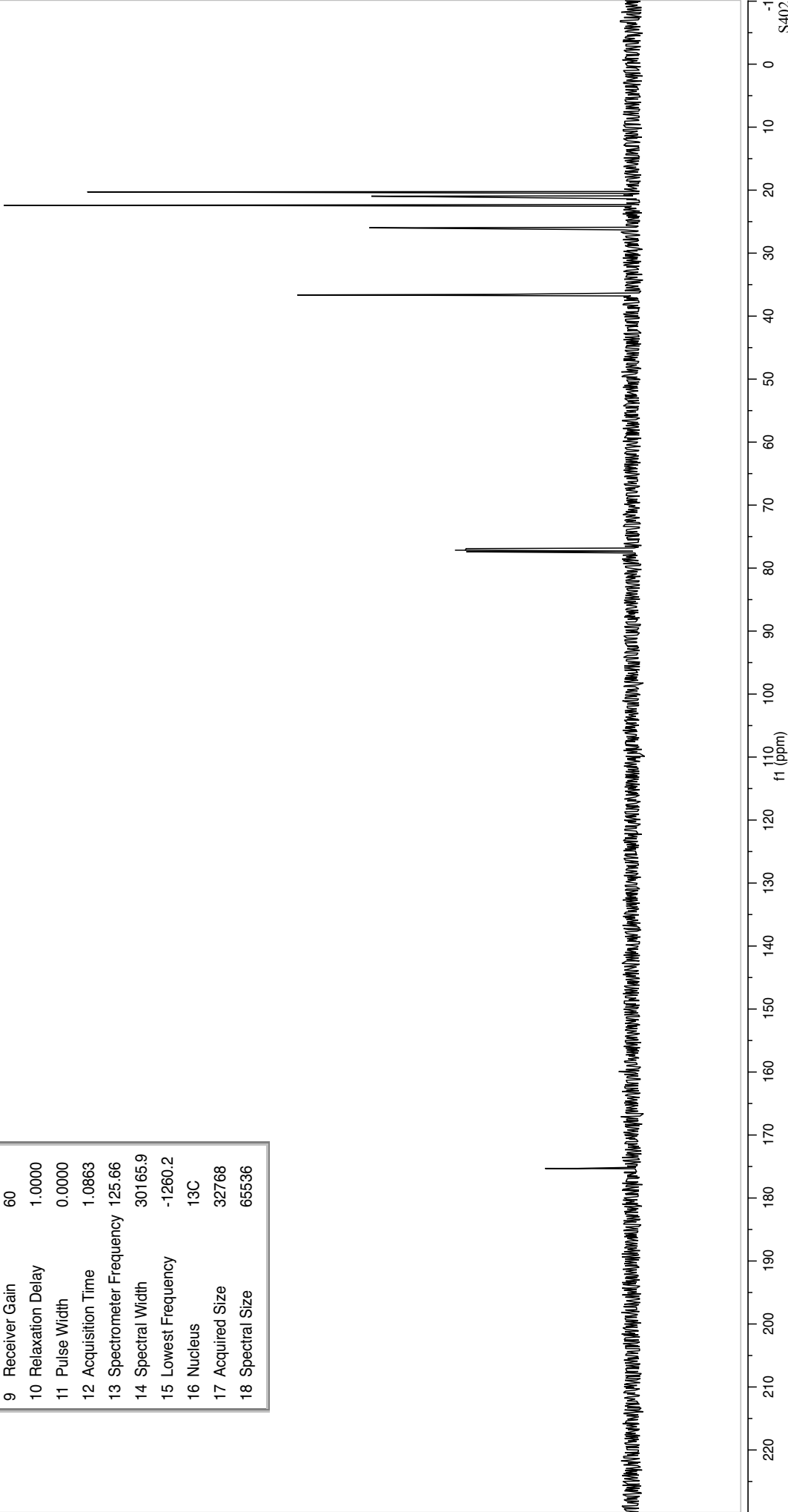
7.26 CDCl₃

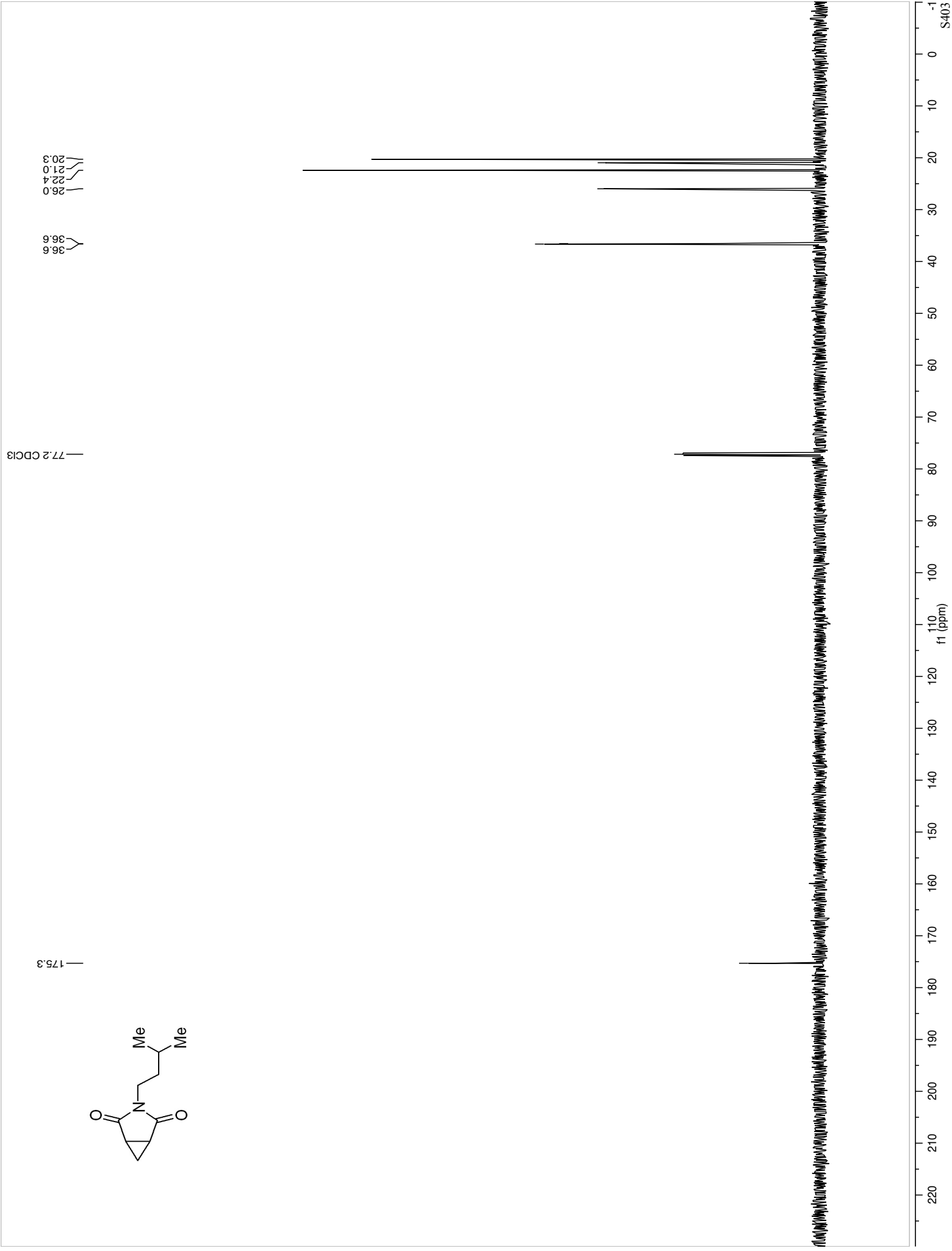
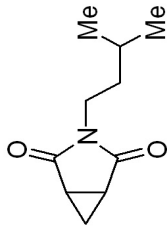


Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	64
9 Receiver Gain	60
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.0863
13 Spectrometer Frequency	125.66
14 Spectral Width	30165.9
15 Lowest Frequency	-1260.2
16 Nucleus	13C
17 Acquired Size	32768
18 Spectral Size	65536



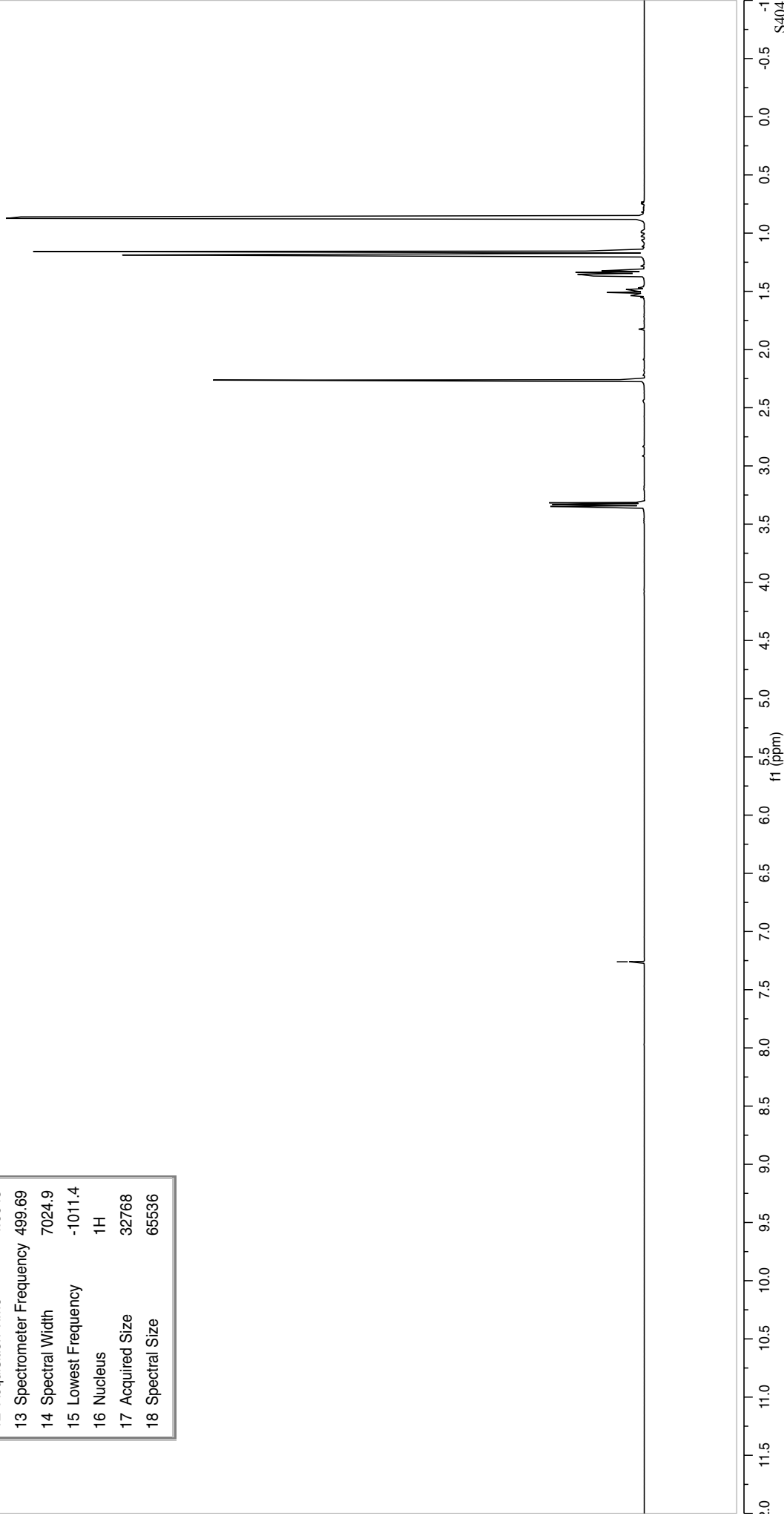
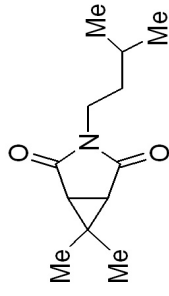
77.2 CDCl3

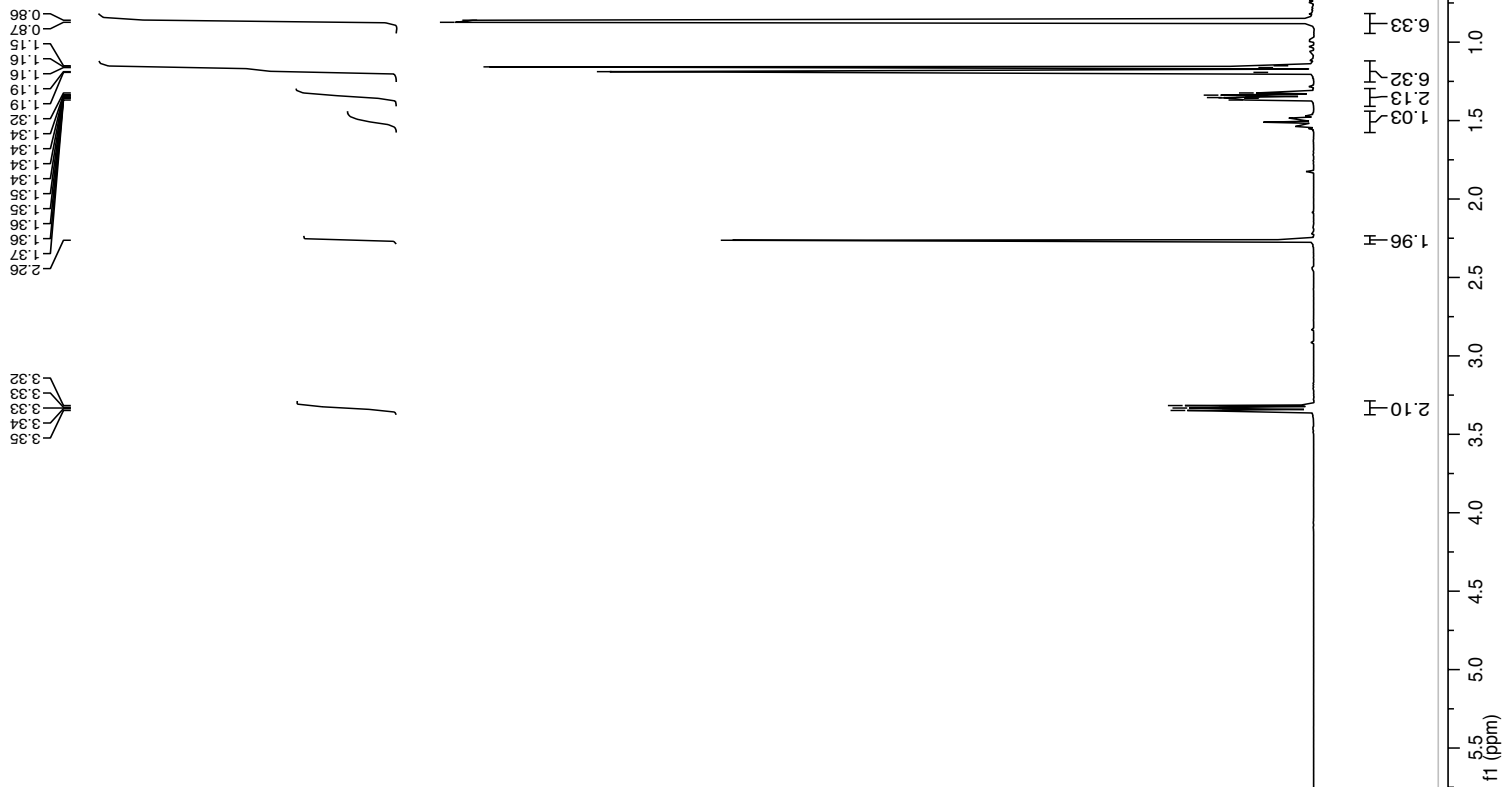
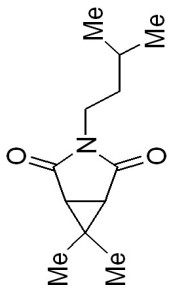




7.26 CDCl3

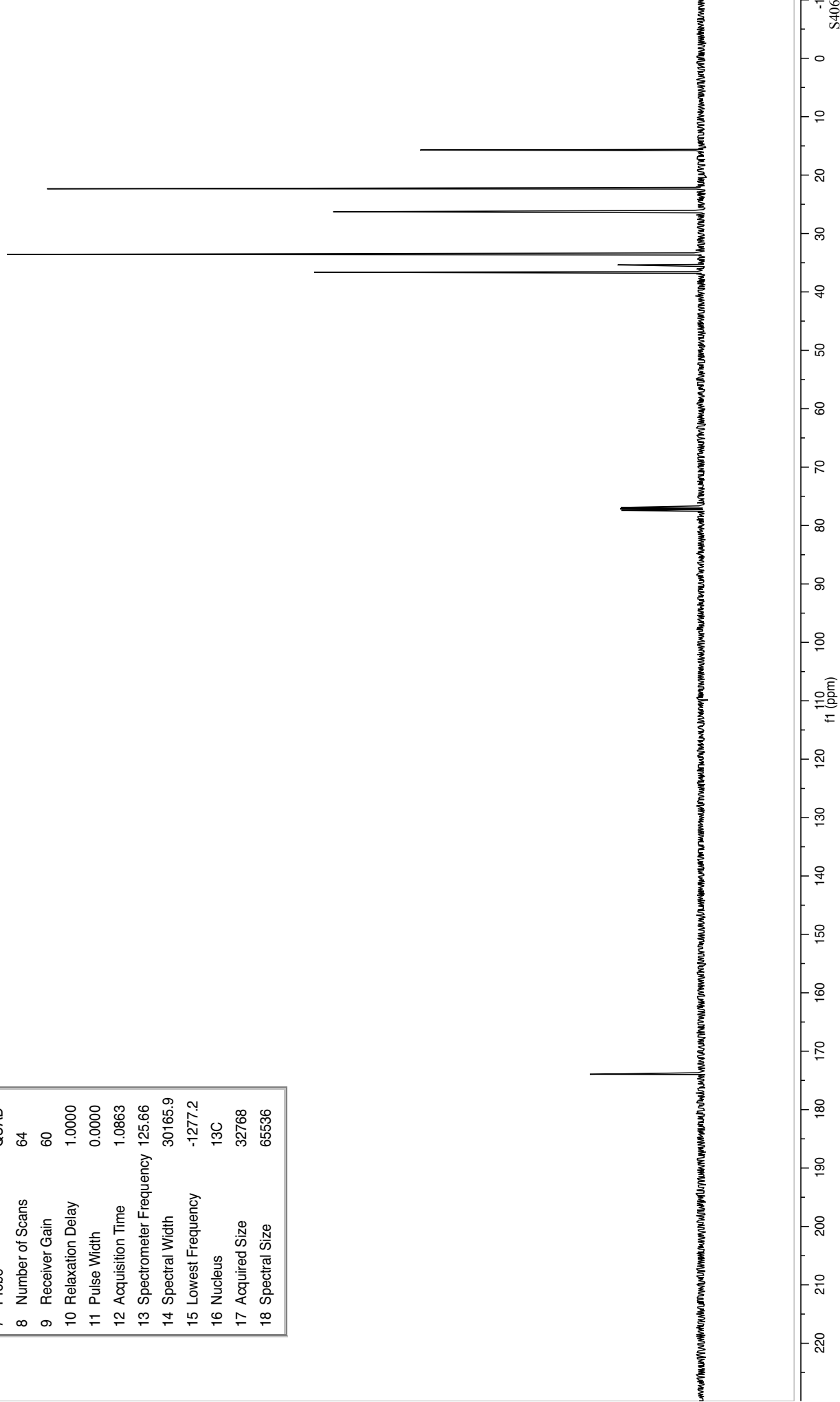
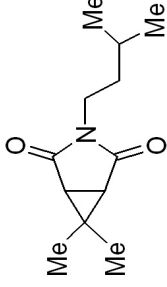
Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	8
9 Receiver Gain	30
10 Relaxation Delay	0.0000
11 Pulse Width	0.0000
12 Acquisition Time	4.6645
13 Spectrometer Frequency	499.69
14 Spectral Width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

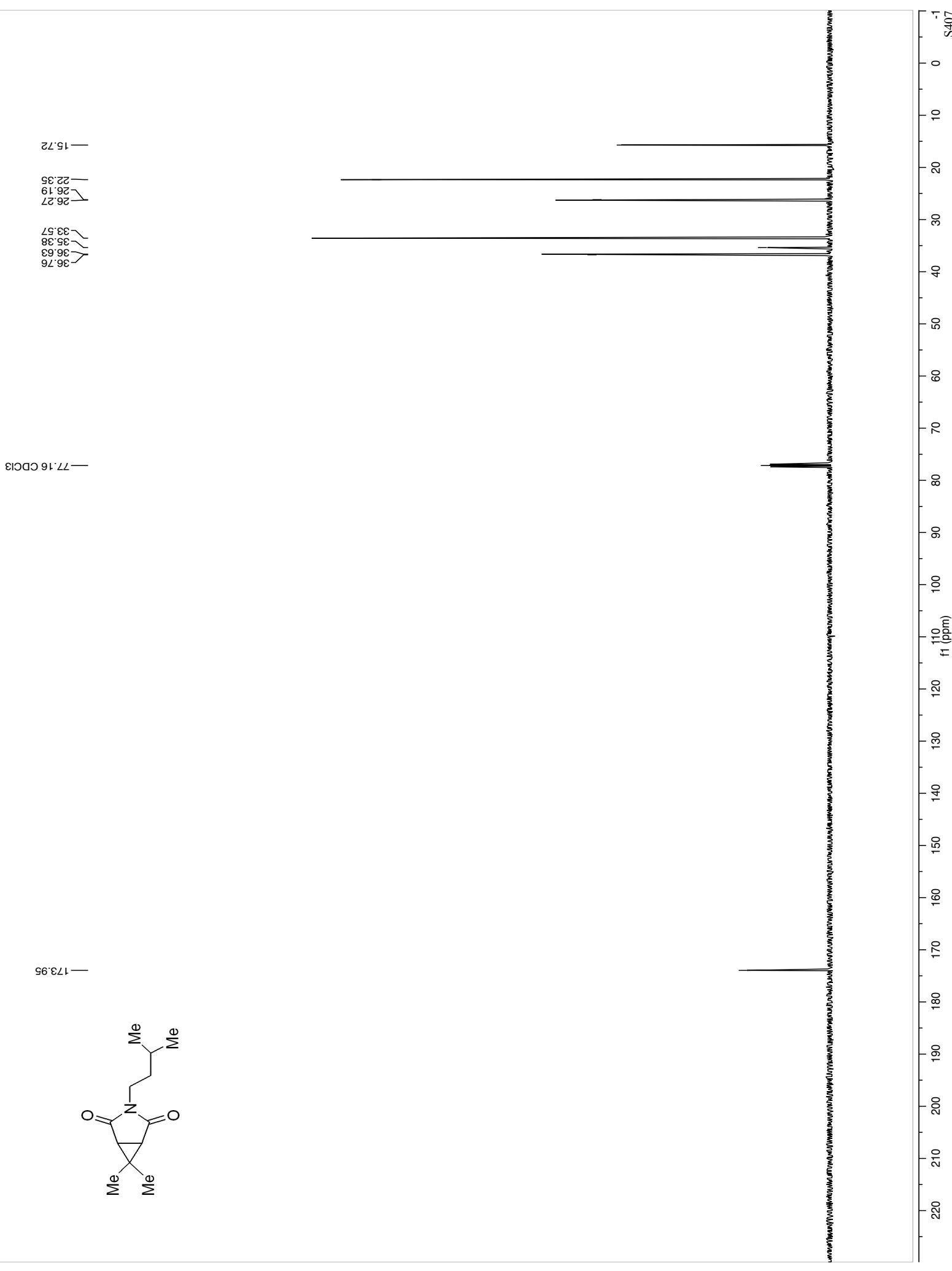




7.26 CDCl₃

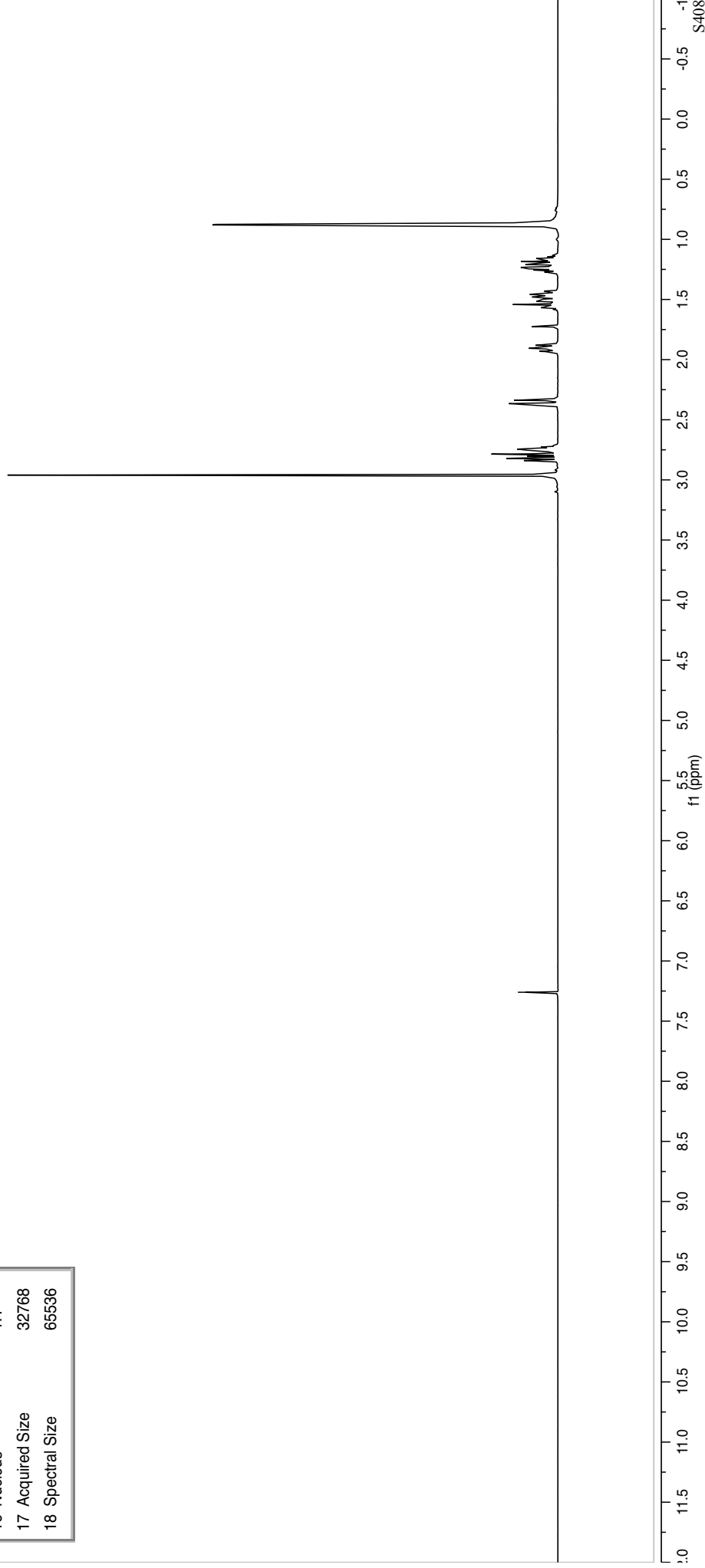
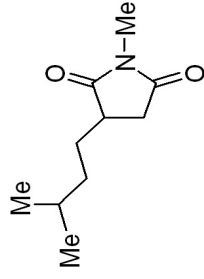
Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	64
9 Receiver Gain	60
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.0863
13 Spectrometer Frequency	125.66
14 Spectral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

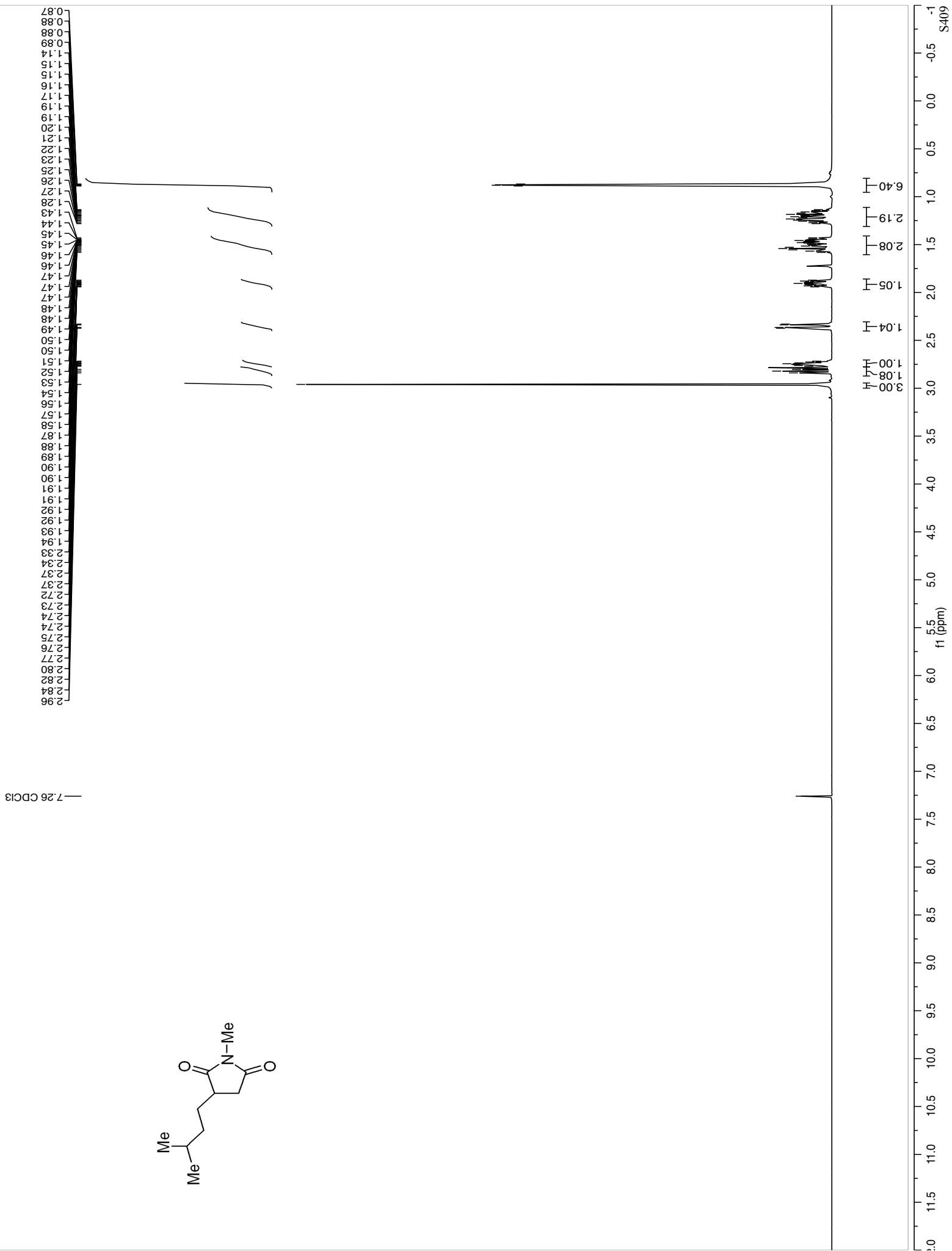
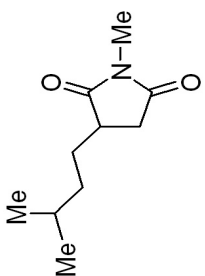


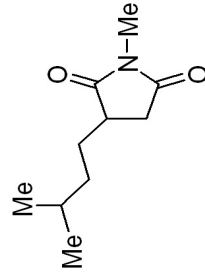


7.3 CDCl3

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	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

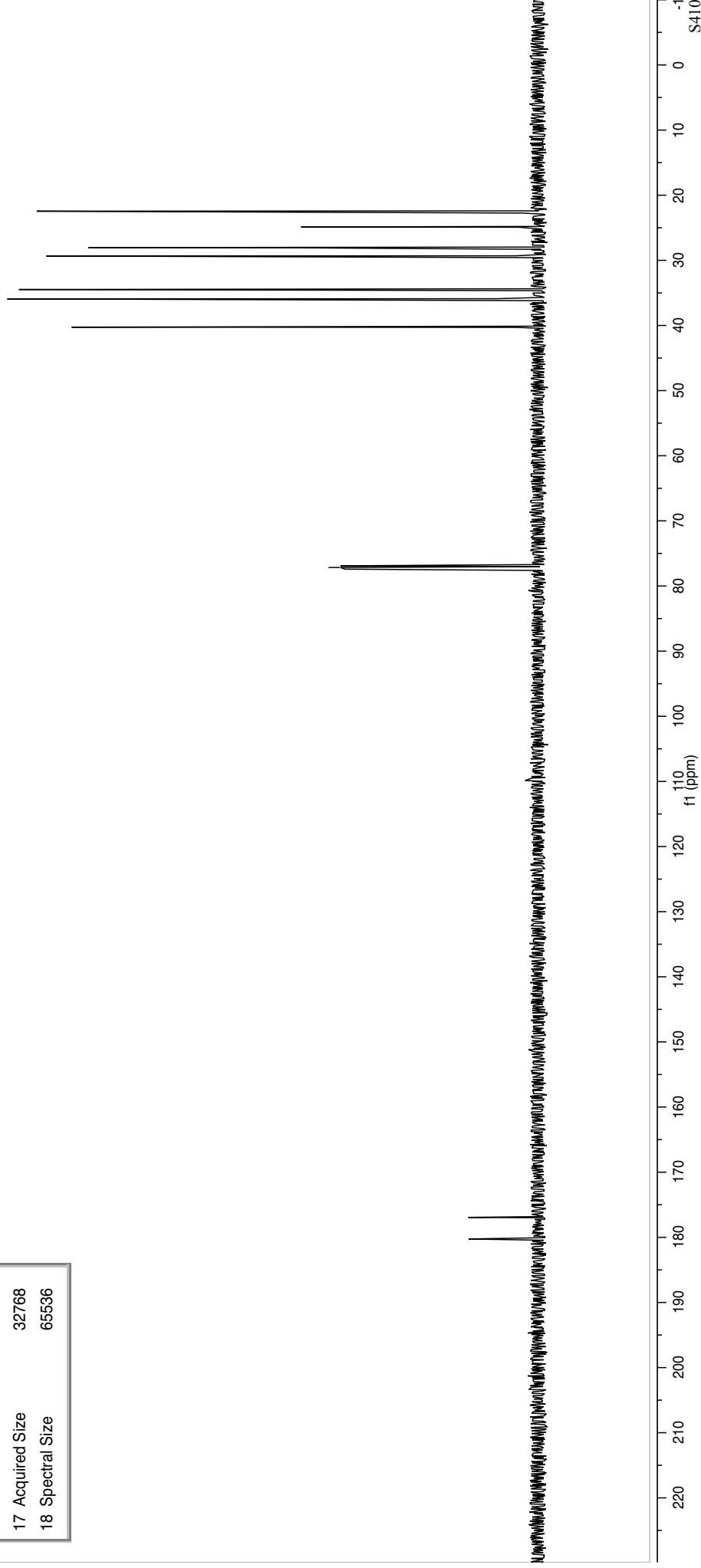


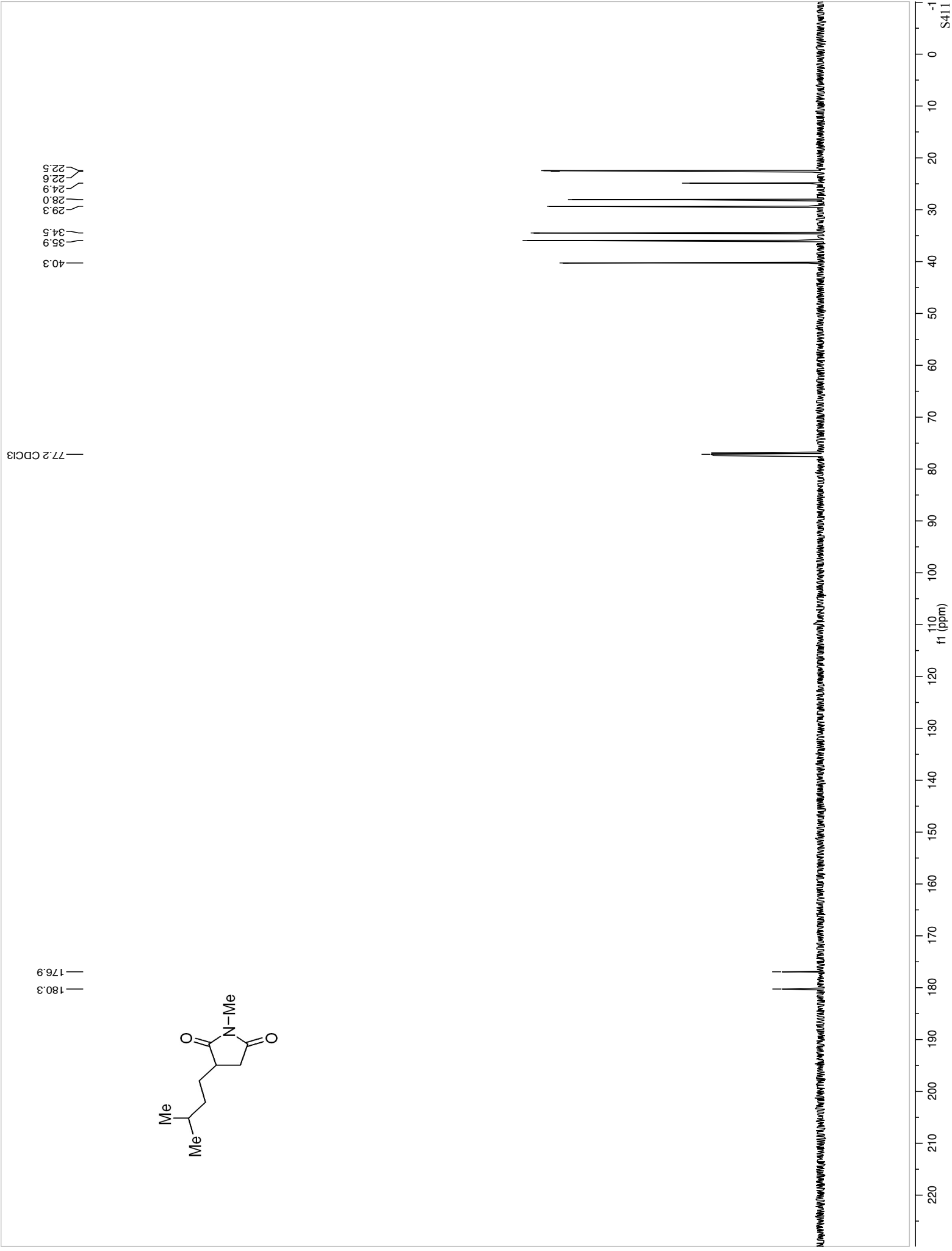
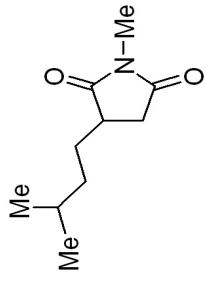




Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	240
9 Receiver Gain	60
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.0863
13 Spectrometer Frequency	125.66
14 Spectral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

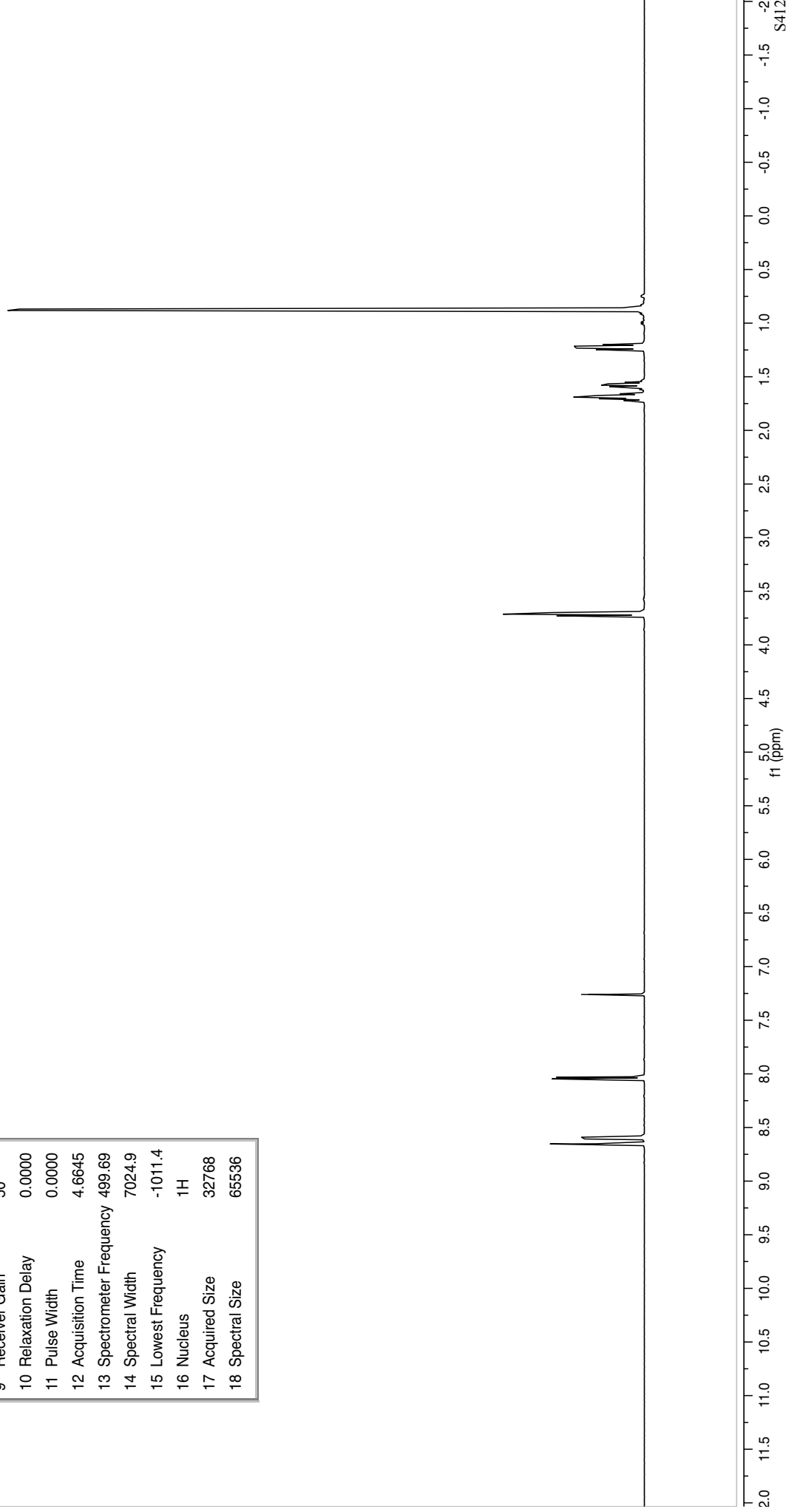
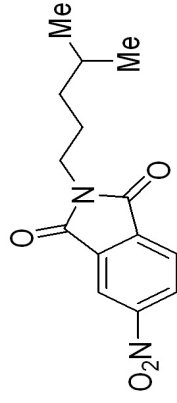
— 77.2 CDCl₃

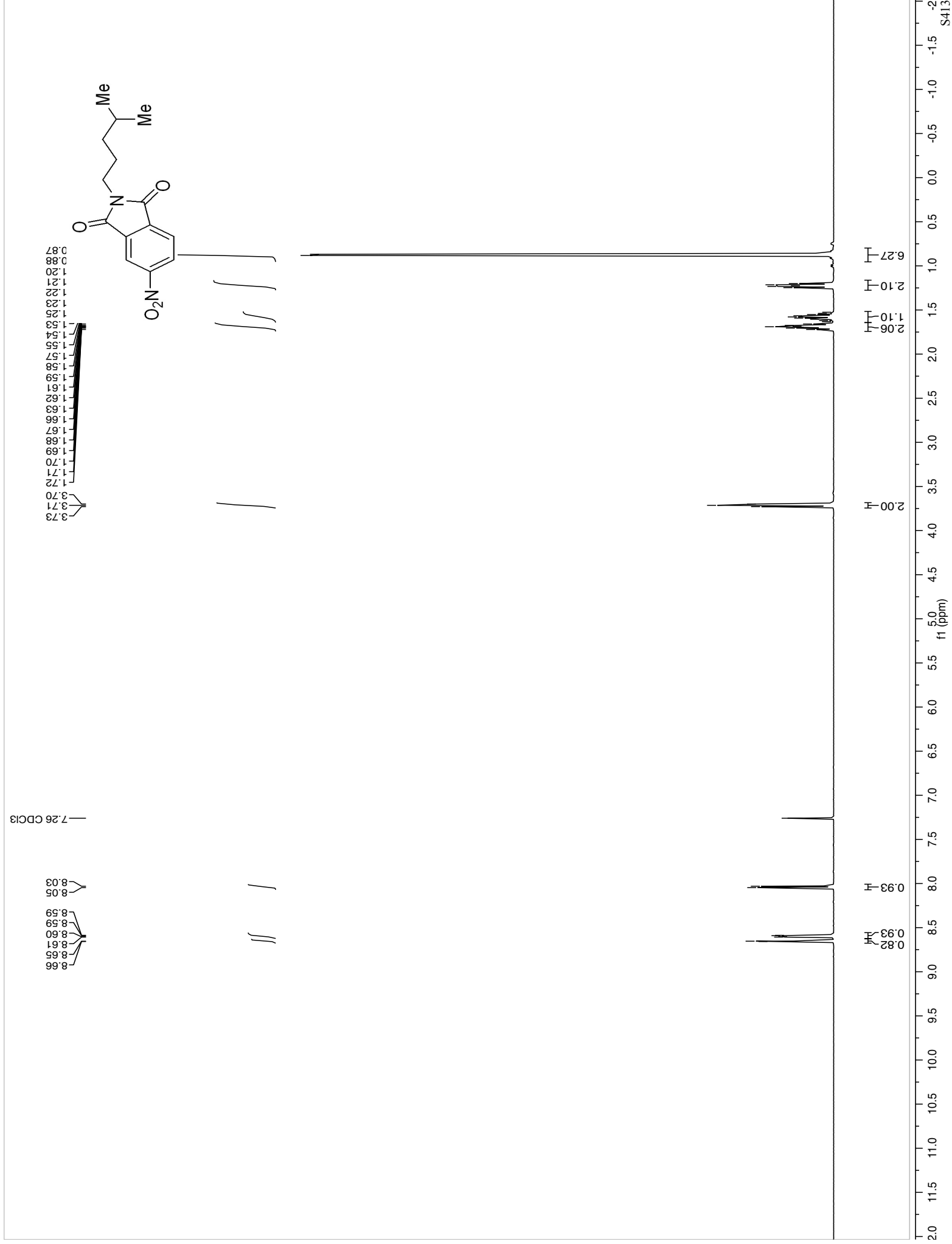




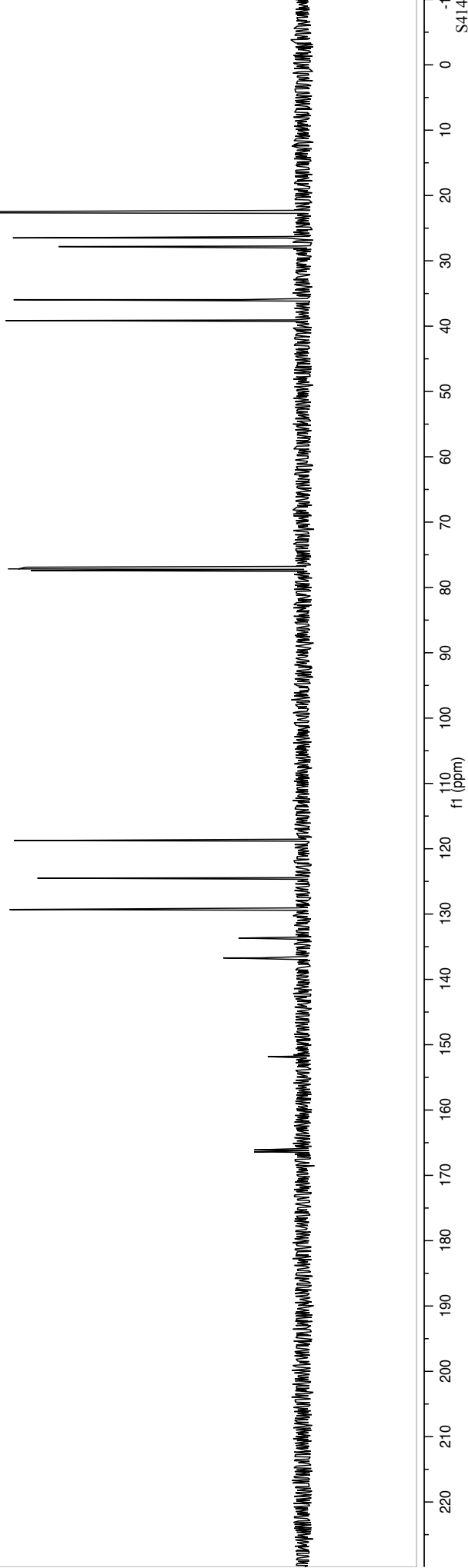
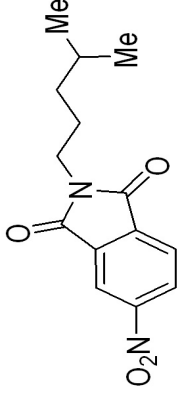
7.26 CDCl3

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	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	1H
17 Acquired Size	32768
18 Spectral Size	65536

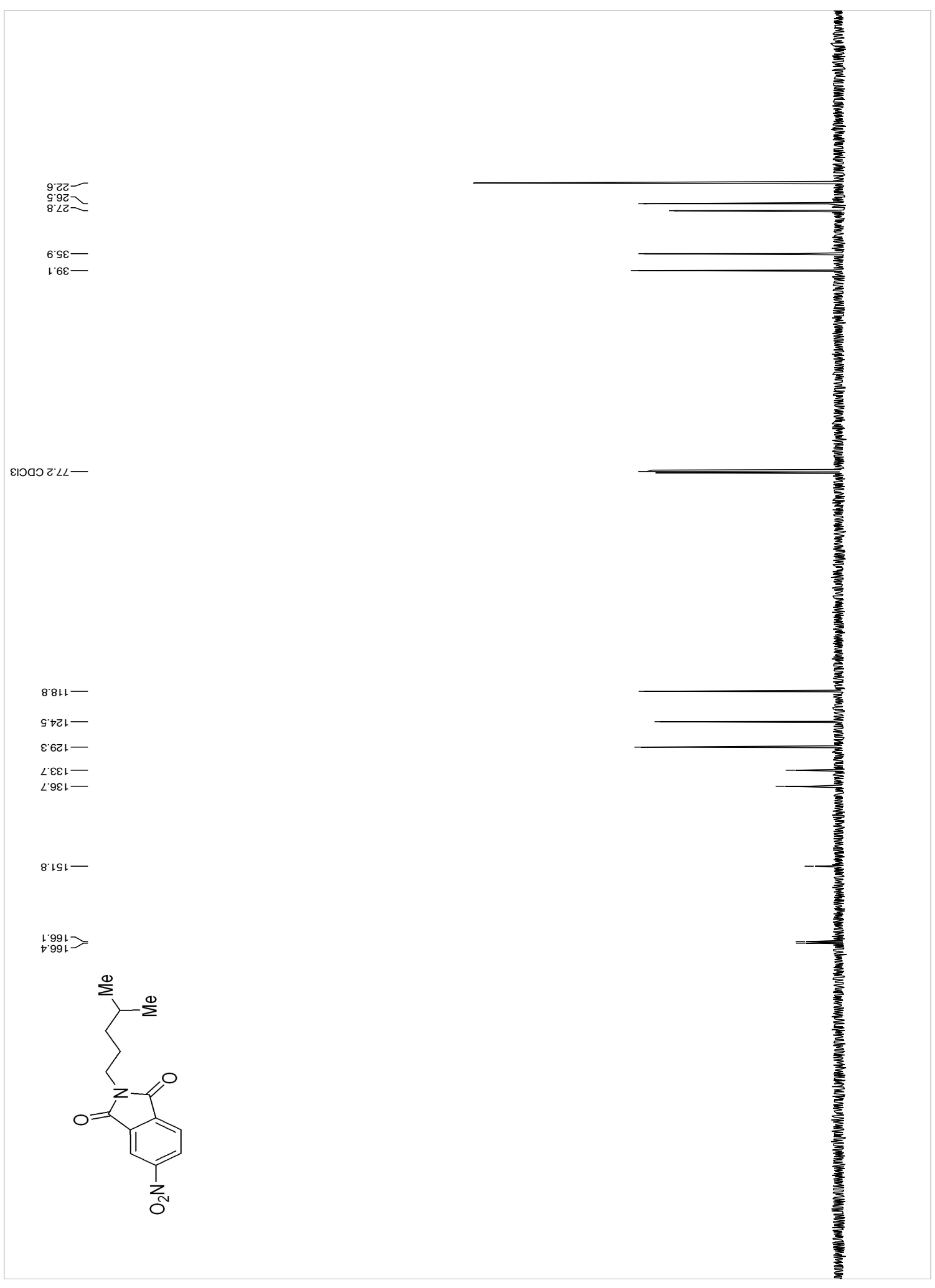




Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	40.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	224
9 Receiver Gain	60
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.0863
13 Spectrometer Frequency	125.66
14 Spectral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

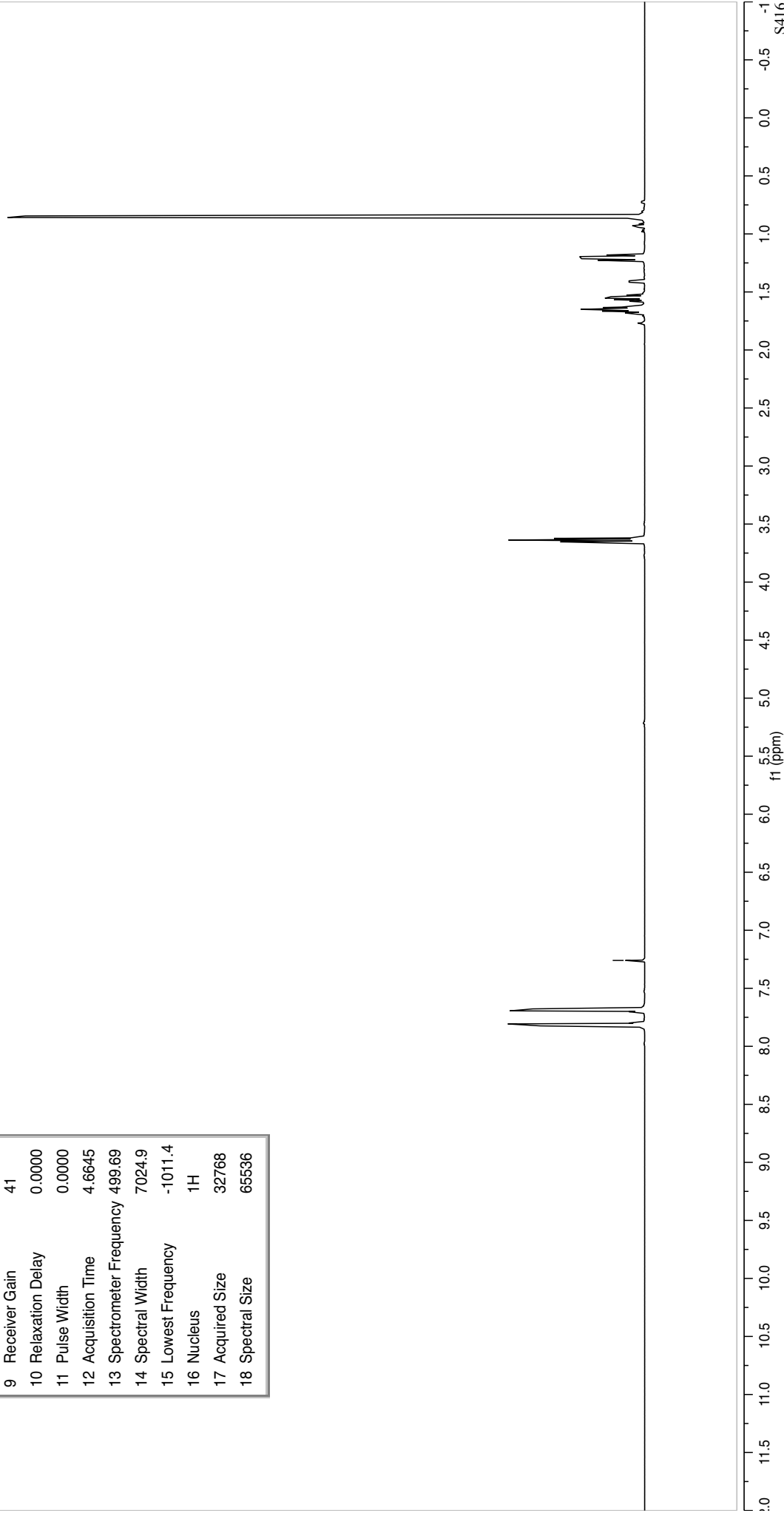
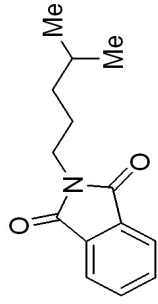


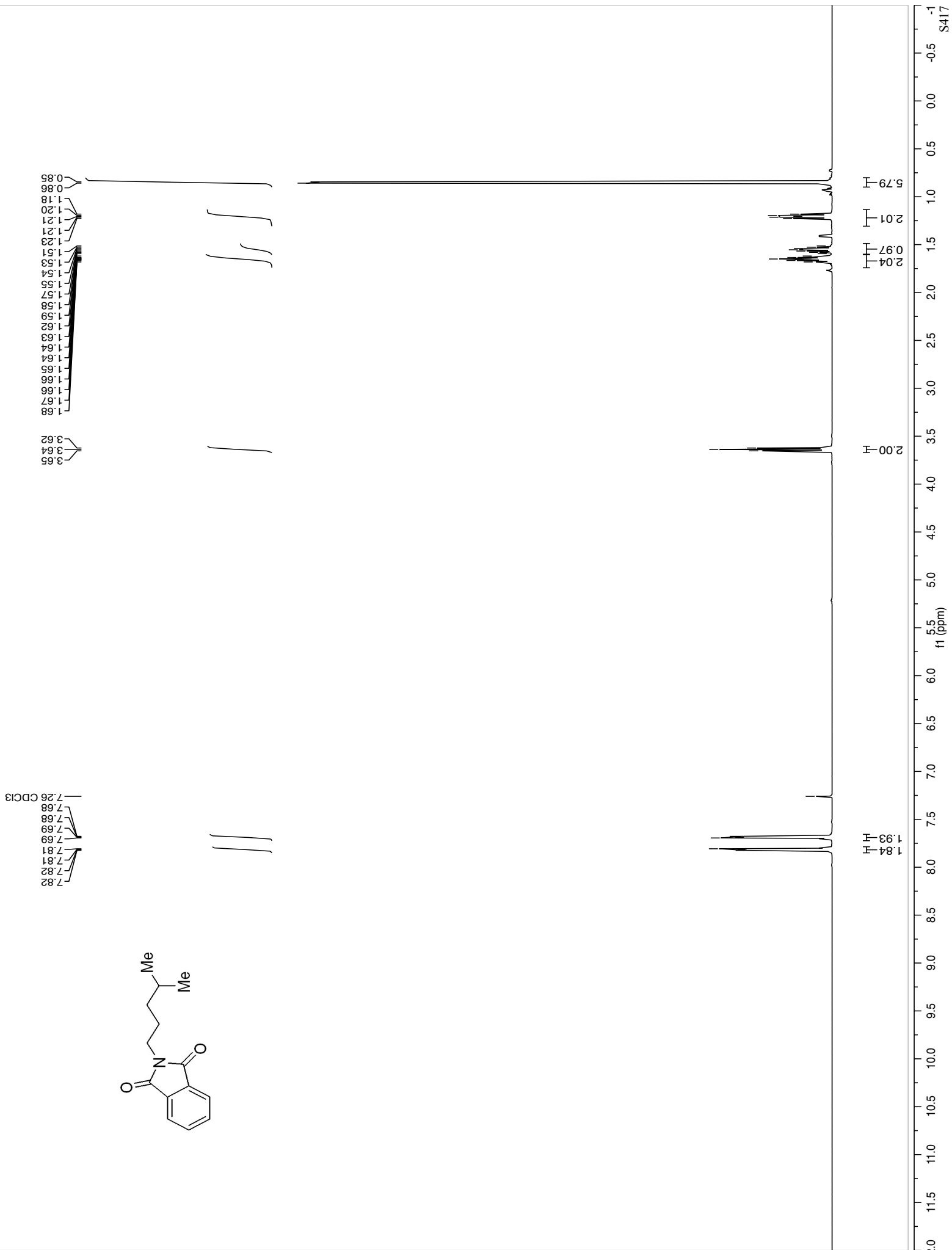
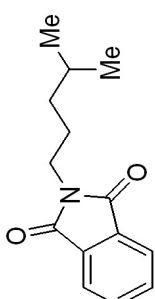
— 77.16 CDCl3

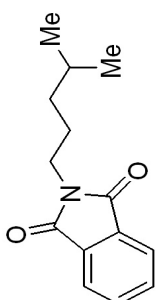
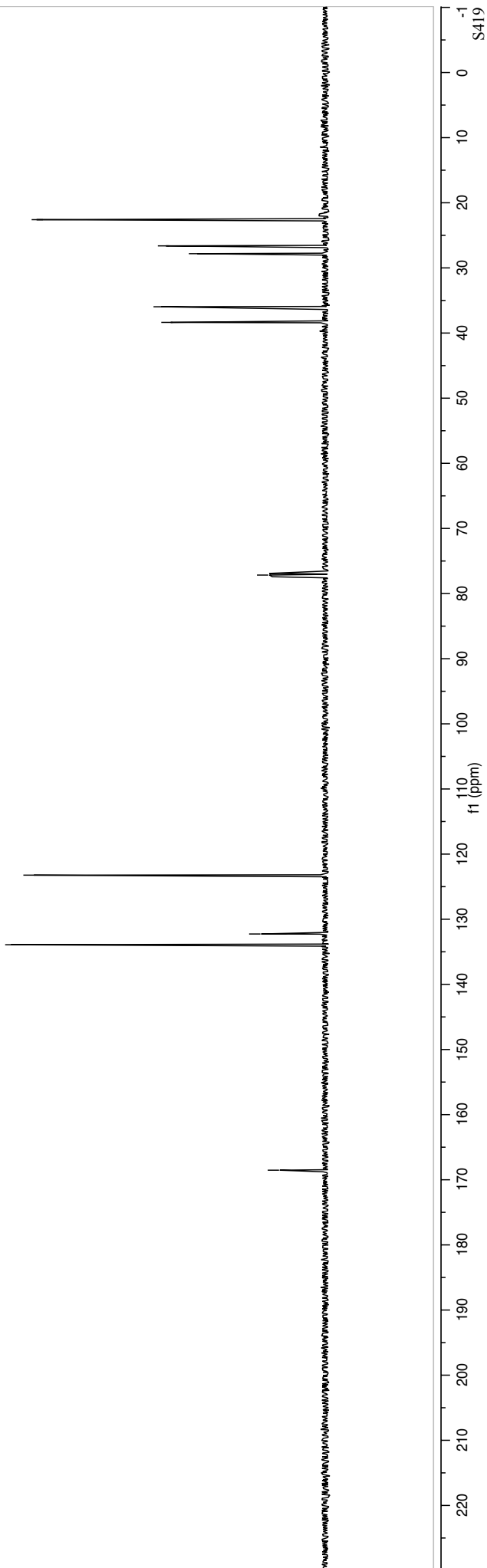


7.26 CDCl₃

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







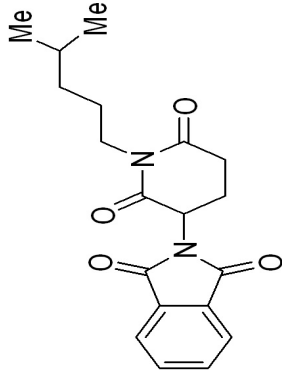
77.2 CDCl₃

38.4
36.0
27.8
26.6
22.6

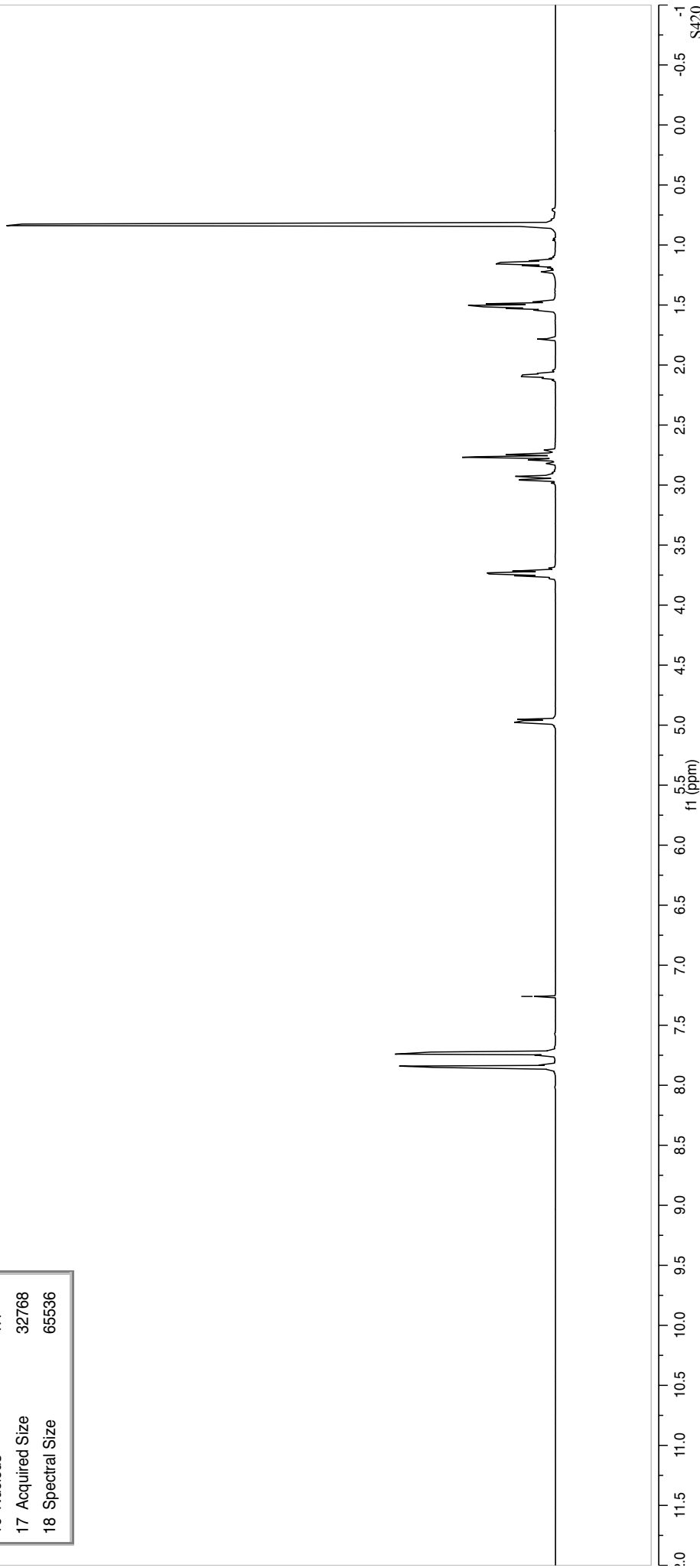
123.2
132.3
133.9

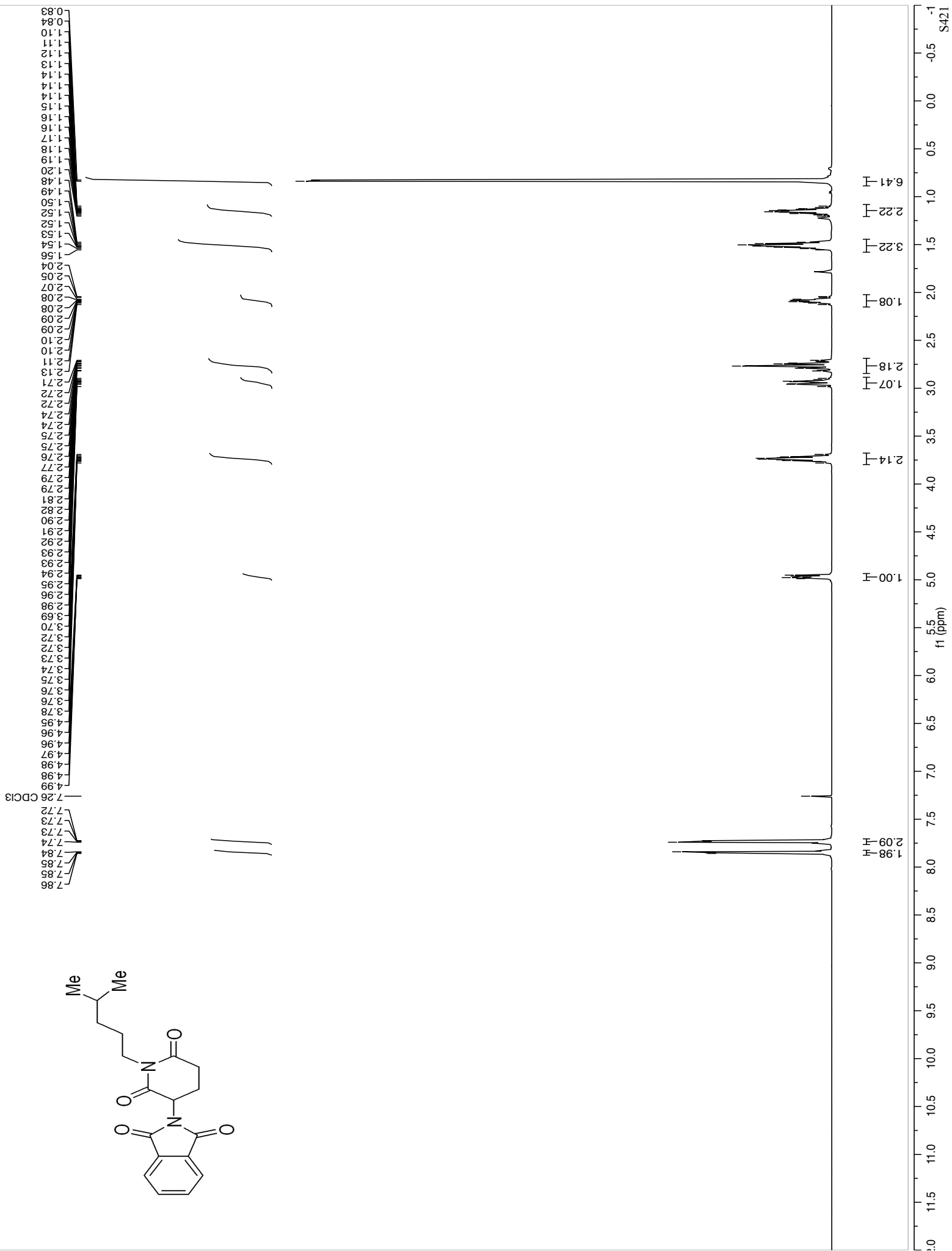
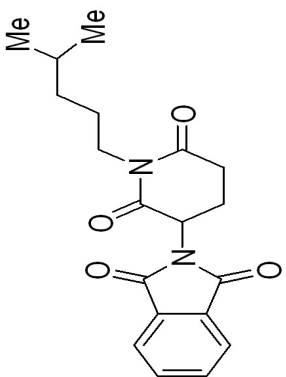
168.5

7.26 CDCl3

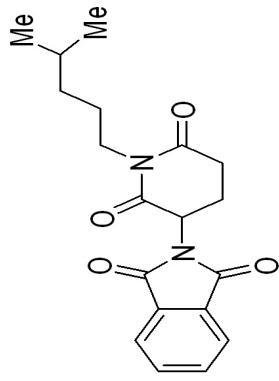


Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	8
9 Receiver Gain	36
10 Relaxation Delay	0.0000
11 Pulse Width	0.0000
12 Acquisition Time	4.6645
13 Spectrometer Frequency	499.69
14 Spectral Width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

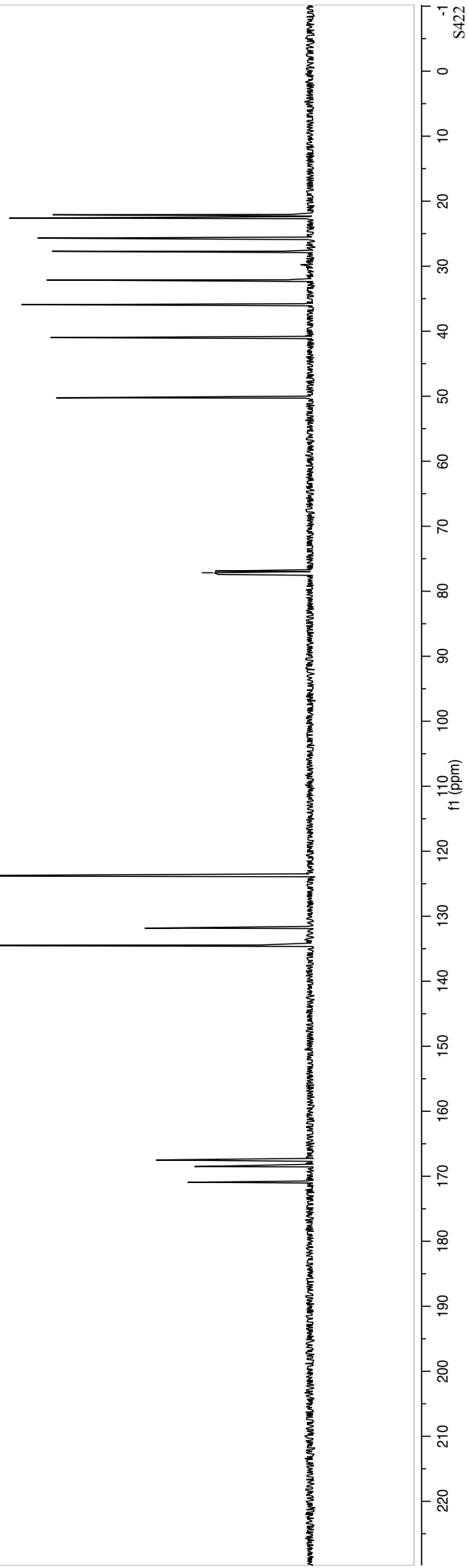


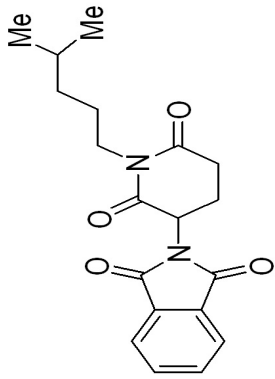


Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	96
9 Receiver Gain	60
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.0863
13 Spectrometer Frequency	125.66
14 Spectral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

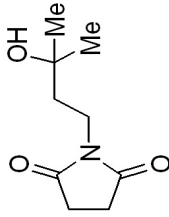


— 77.2 CDCl3

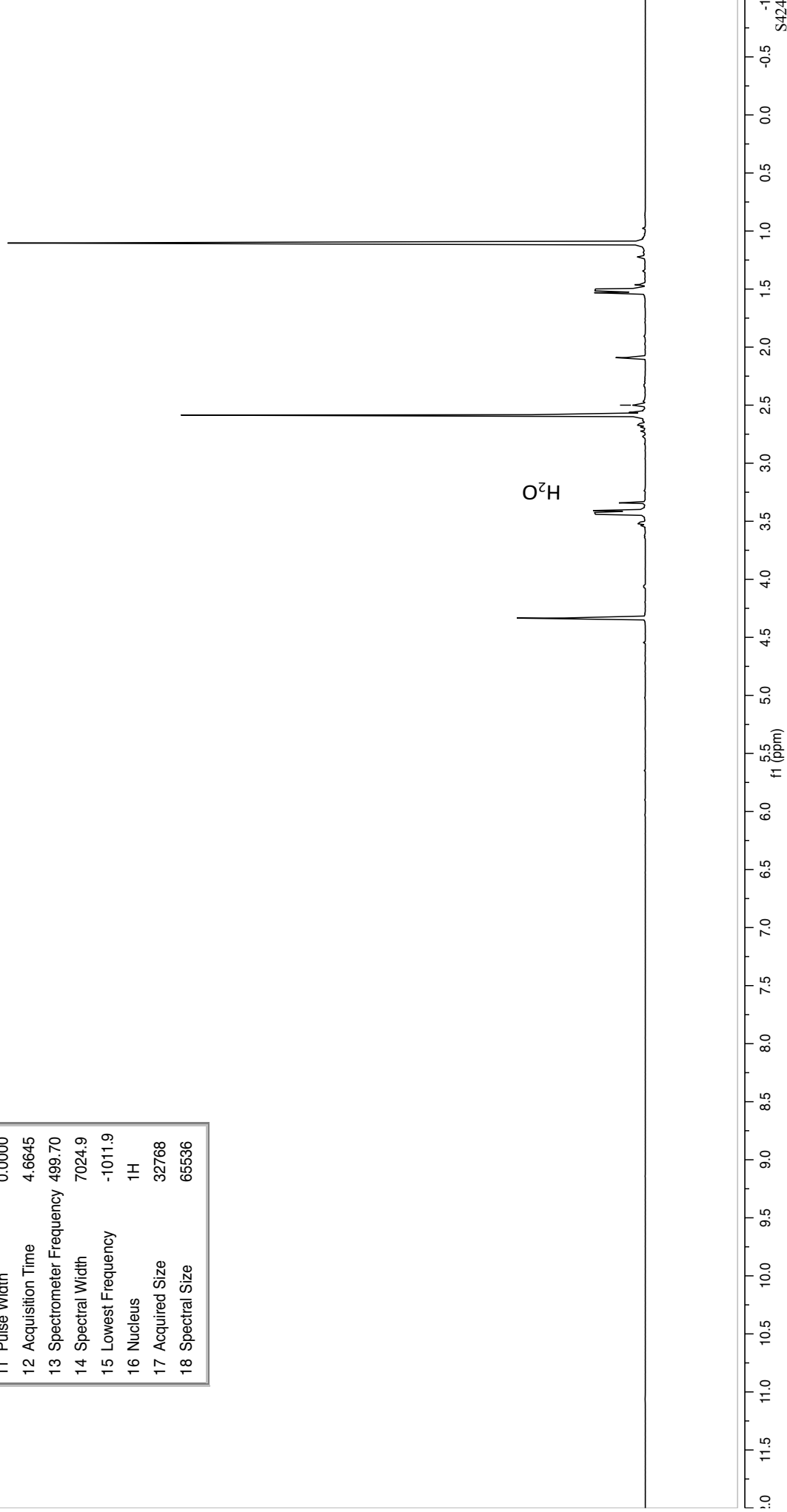


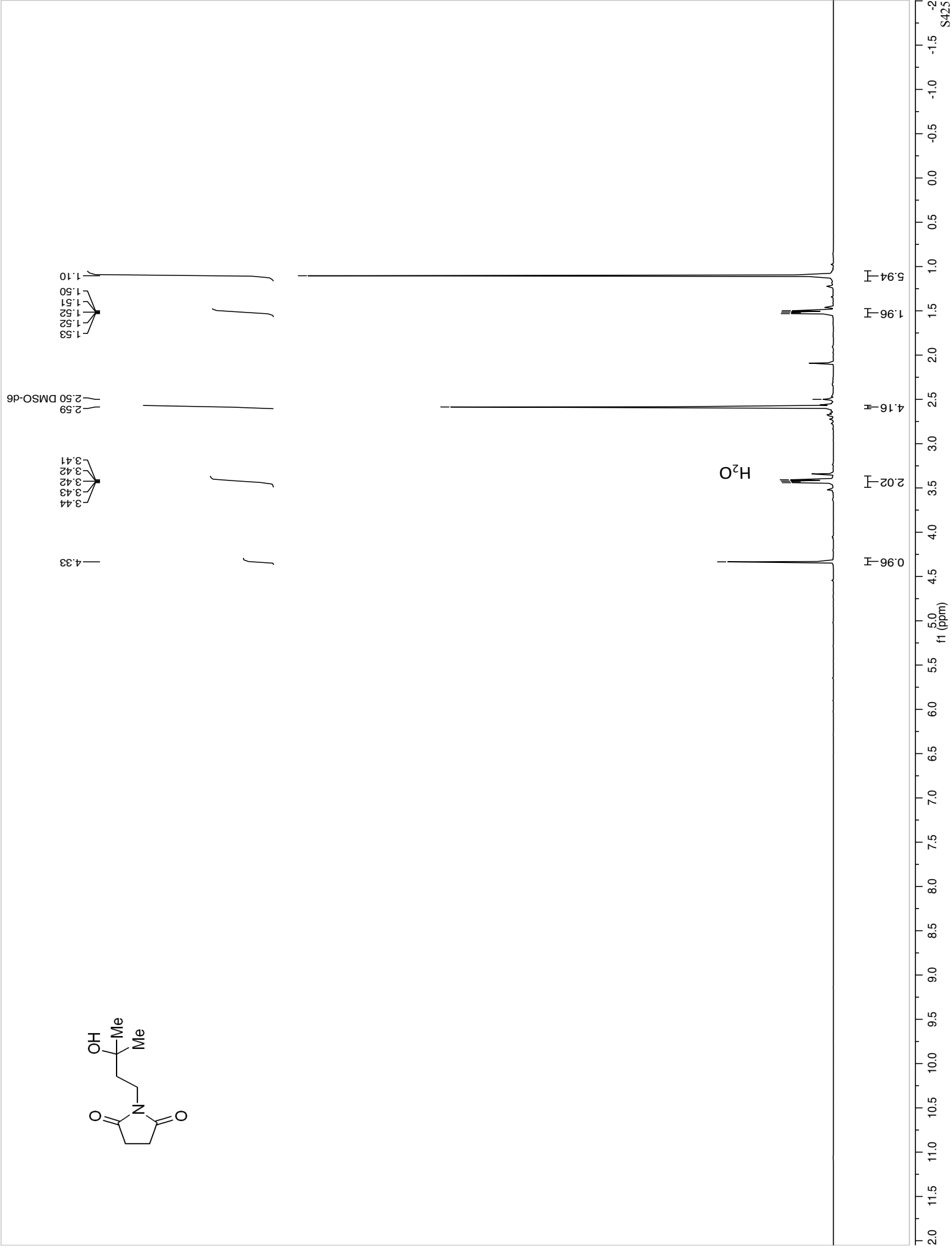
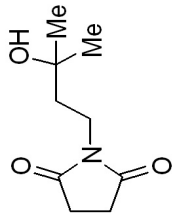


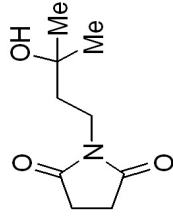
Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	DMSO
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	8
9 Receiver Gain	36
10 Relaxation Delay	0.0000
11 Pulse Width	0.0000
12 Acquisition Time	4.6645
13 Spectrometer Frequency	499.70
14 Spectral Width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



— 2.50 DMSO-d6

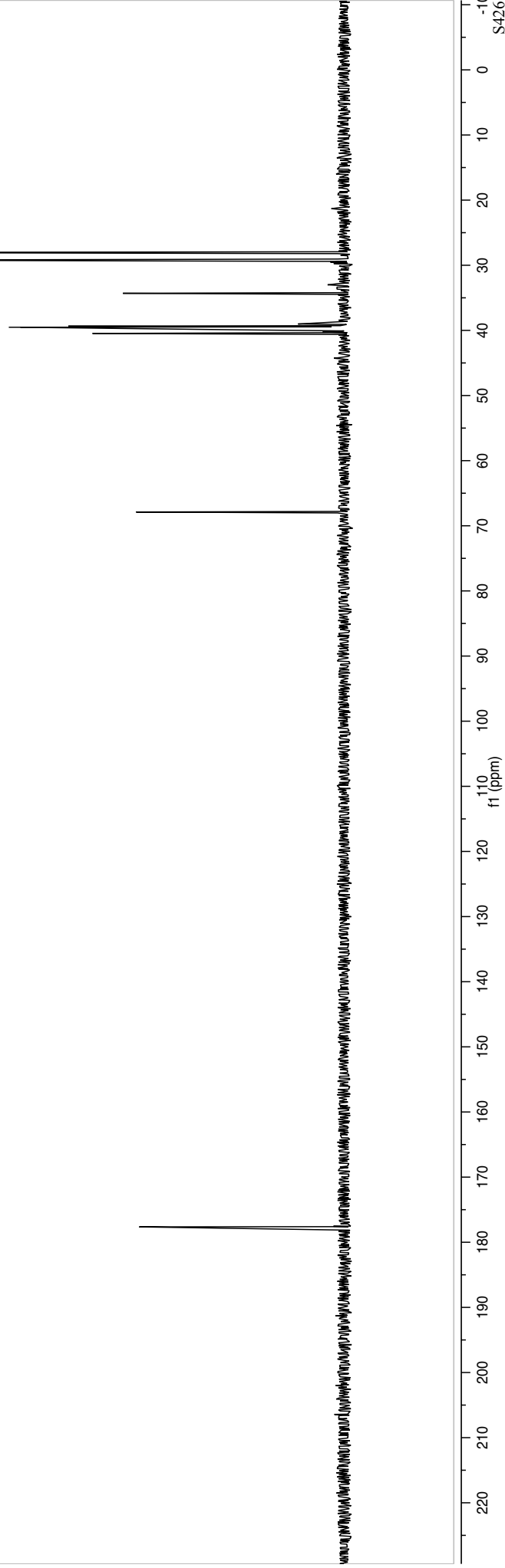


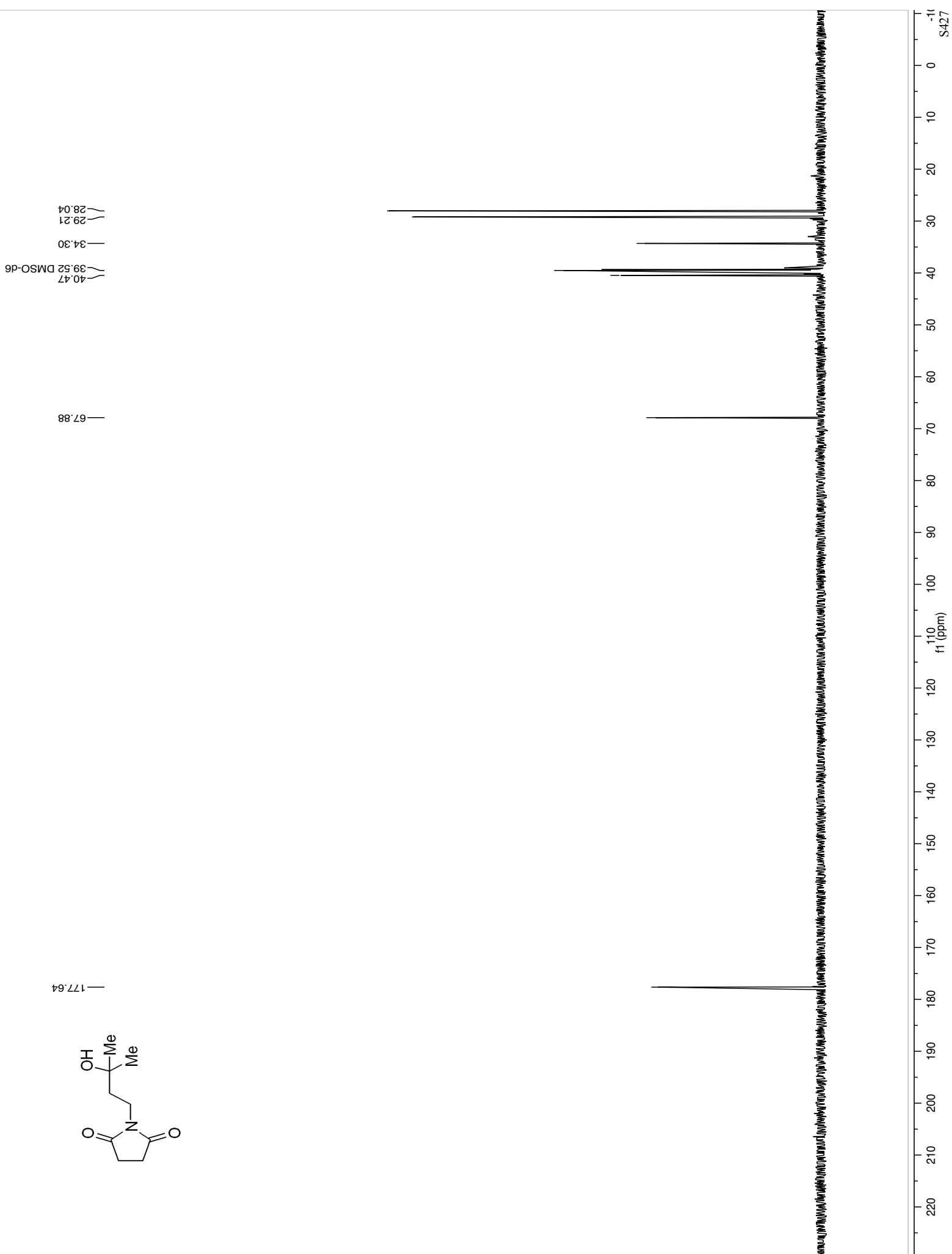


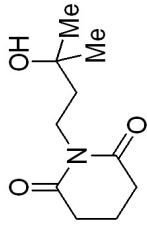


— 39.52 DMSO-d6

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



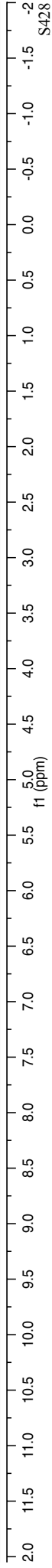


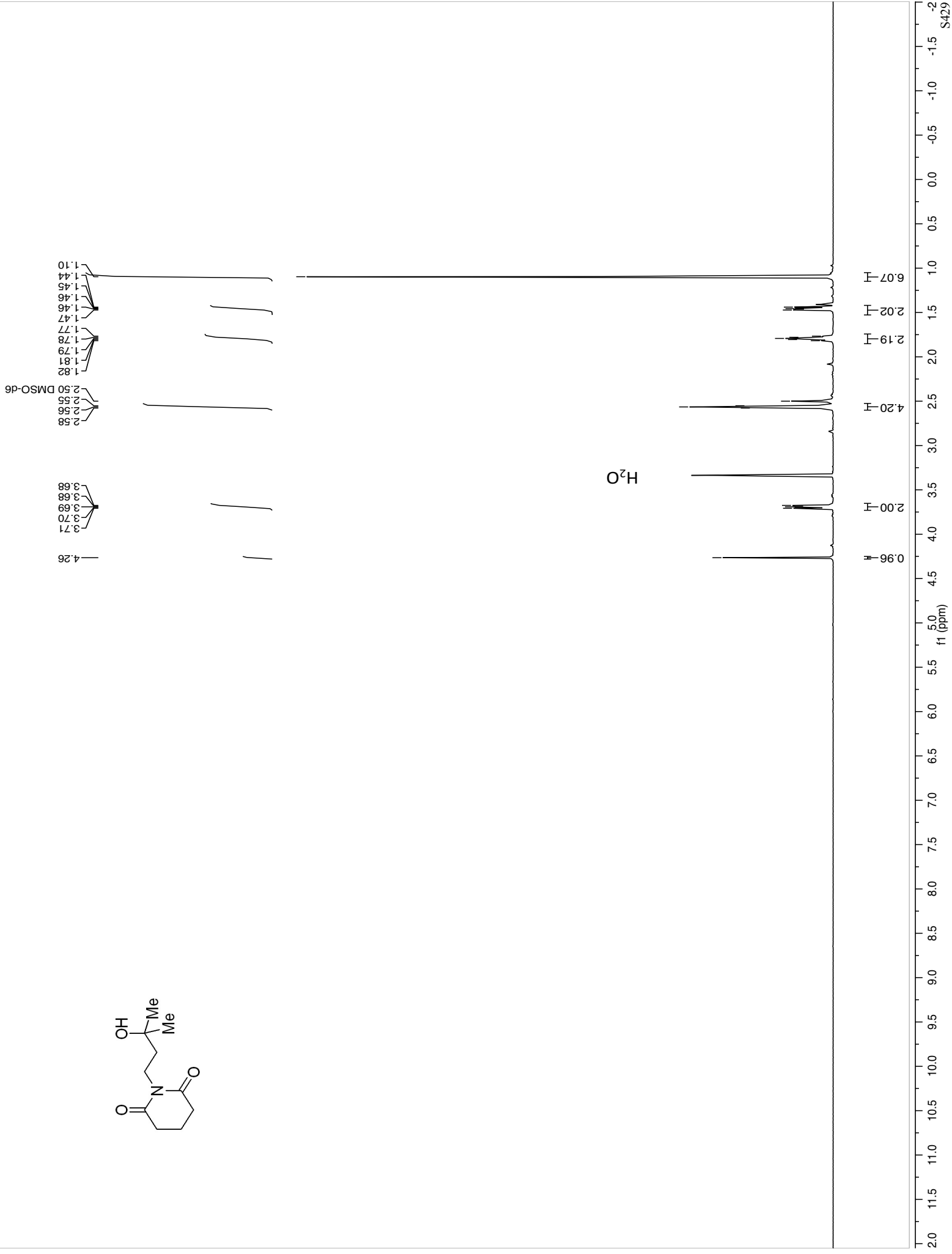
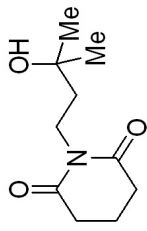


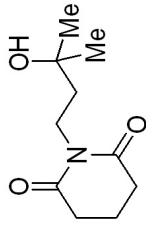
— 2.50 DMSO-d6

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	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

H₂O

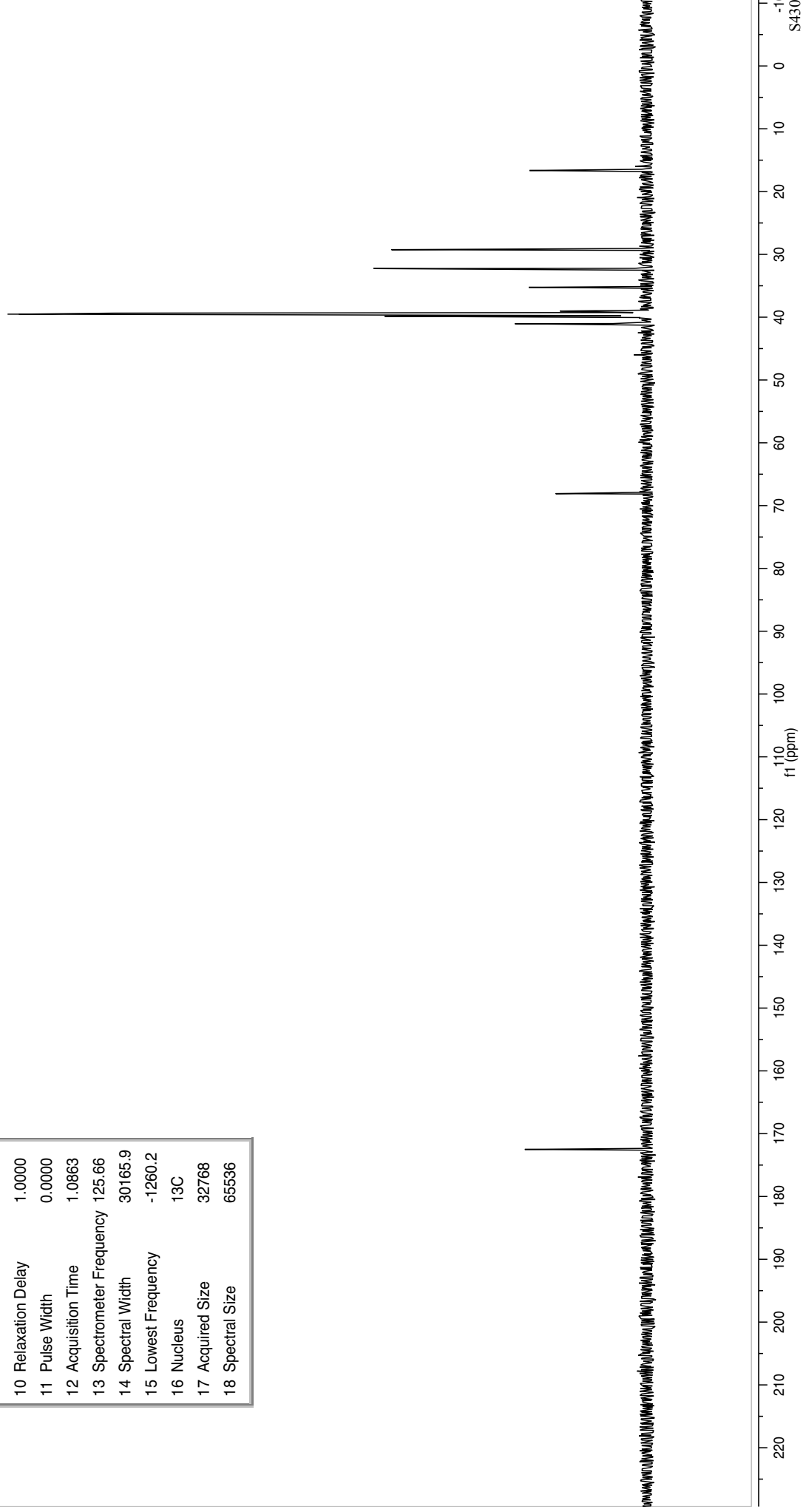


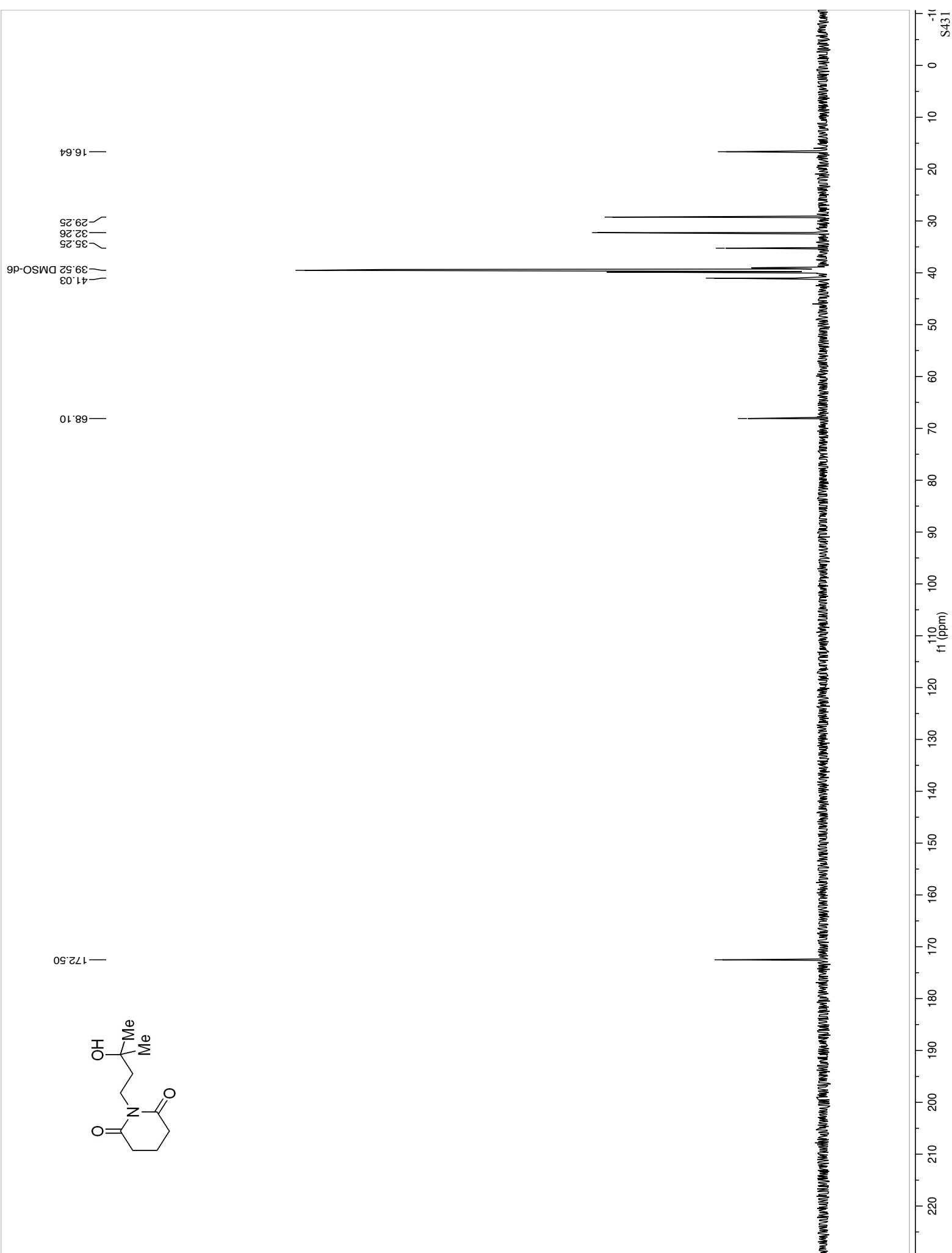




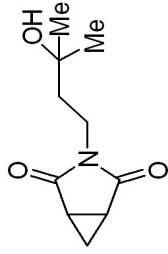
Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	DMSO
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	256
9 Receiver Gain	60
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.0863
13 Spectrometer Frequency	125.66
14 Spectral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

39.52 DMSO-d6

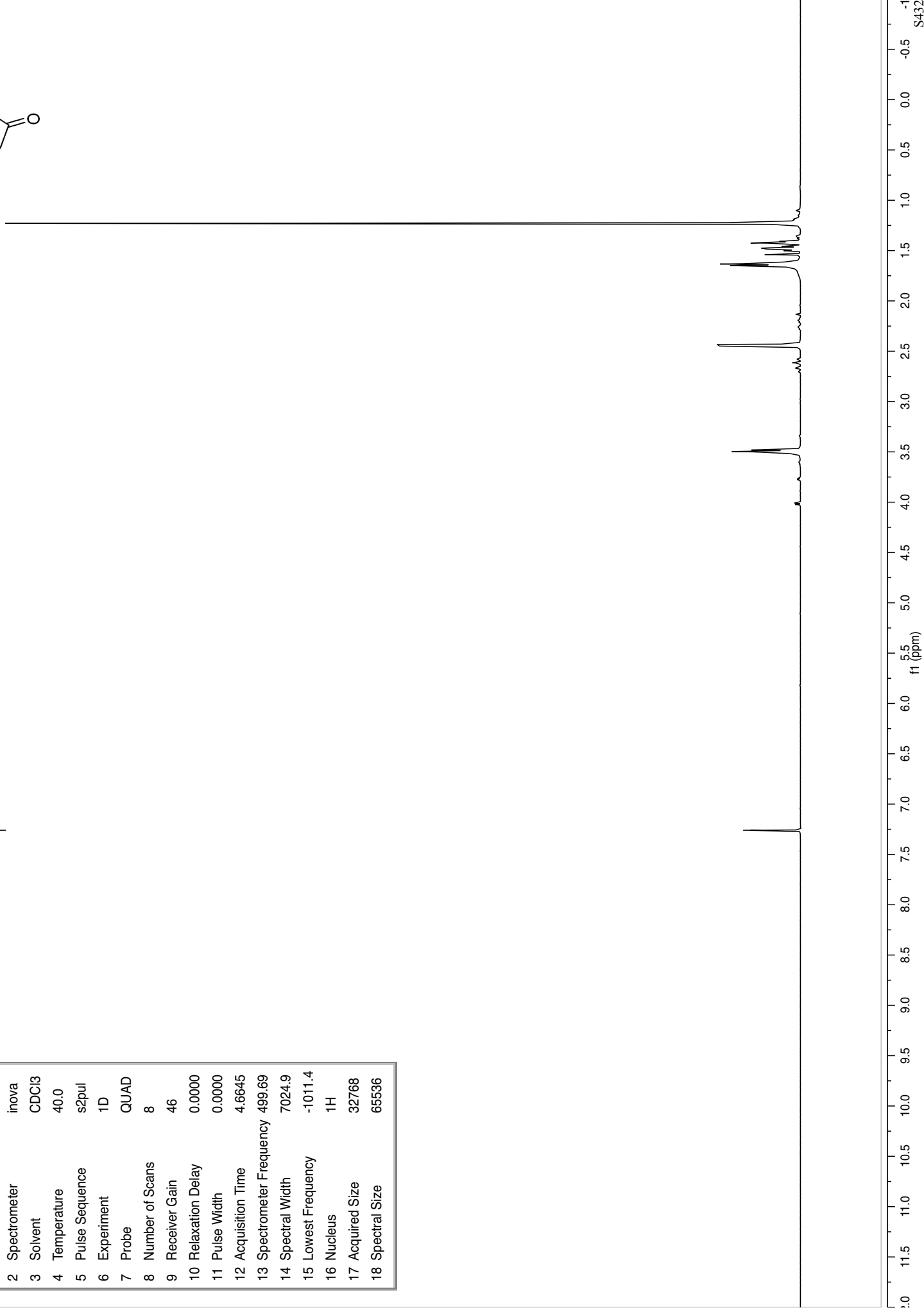




7.3 CDCl3



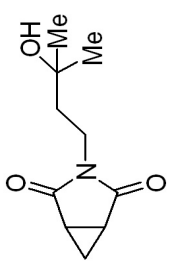
Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	40.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	8
9 Receiver Gain	46
10 Relaxation Delay	0.0000
11 Pulse Width	0.0000
12 Acquisition Time	4.6645
13 Spectrometer Frequency	499.69
14 Spectral Width	7024.9
15 Lowest Frequency	-1011.4
16 Nucleus	1H
17 Acquired Size	32768
18 Spectral Size	65536



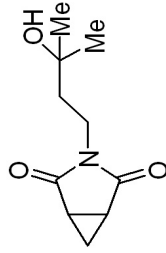
S433

5.99 H
3.02 H
1.00 H
1.90 H
1.93 H

1.23
1.41
1.42
1.42
1.43
1.46
1.47
1.48
1.48
1.49
1.50
1.62
1.63
1.65
2.43
2.44
2.45
2.46
3.48
3.51

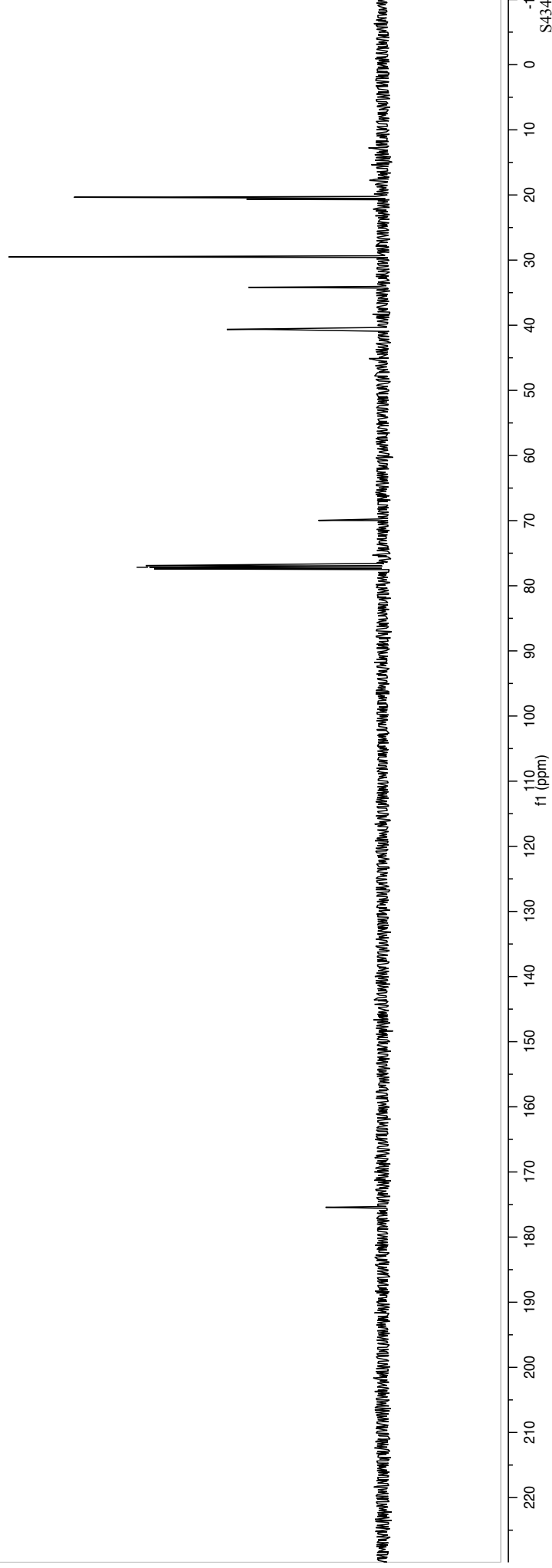


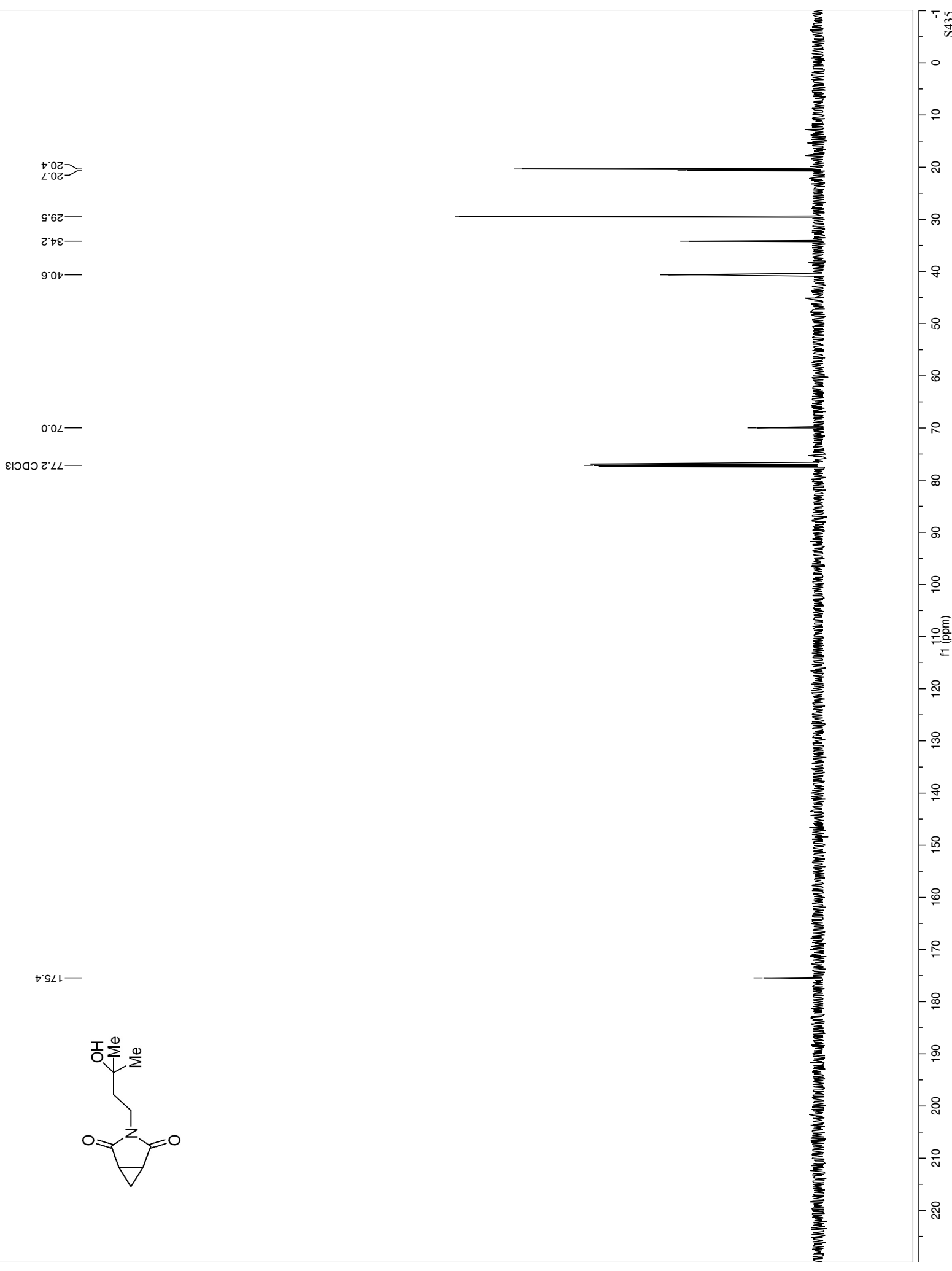
7.26 CDCl₃



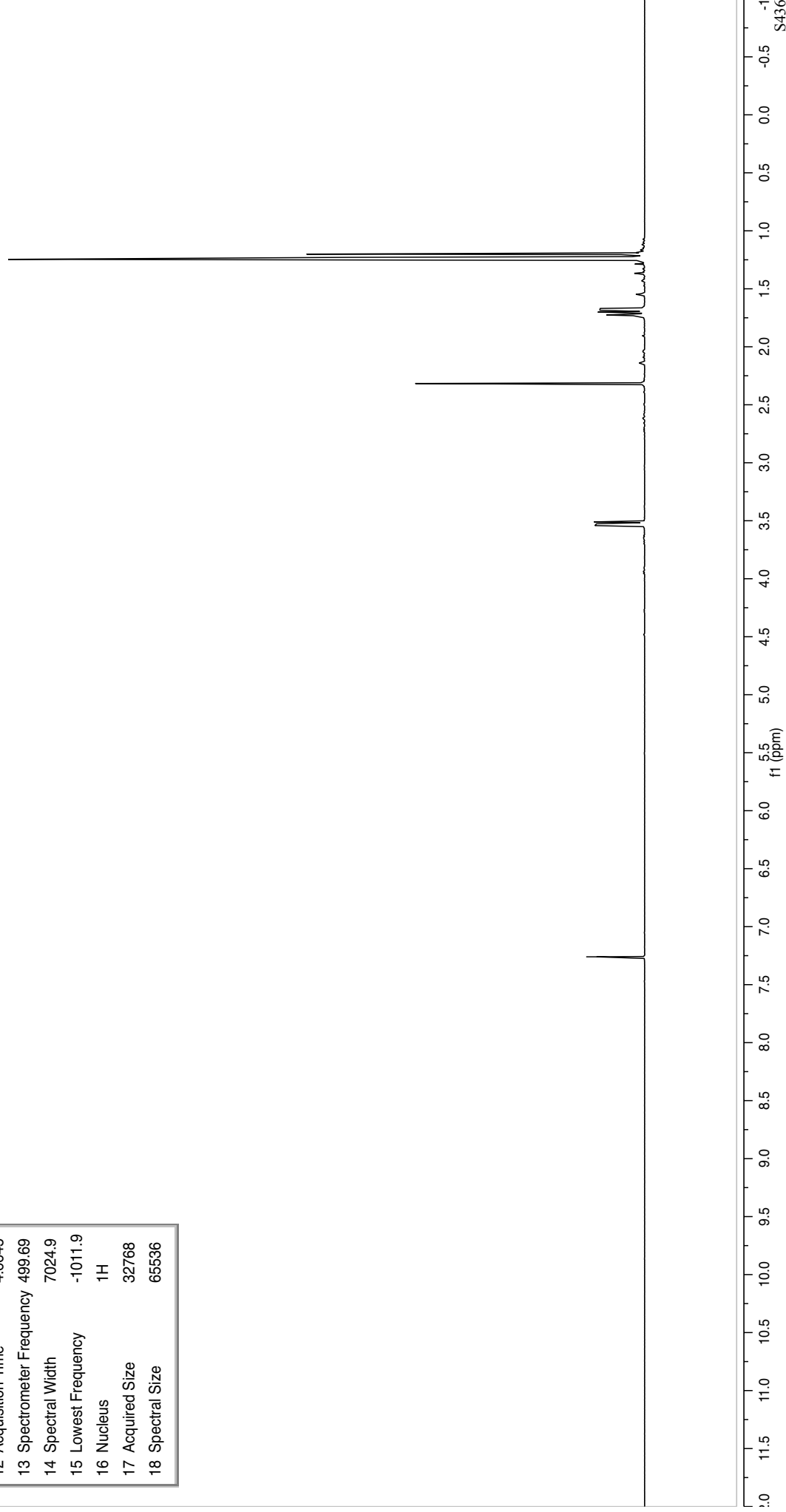
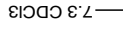
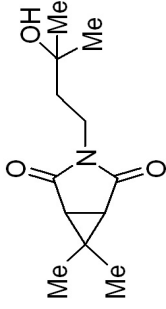
Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	40.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	192
9 Receiver Gain	60
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.0863
13 Spectrometer Frequency	125.66
14 Spectral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

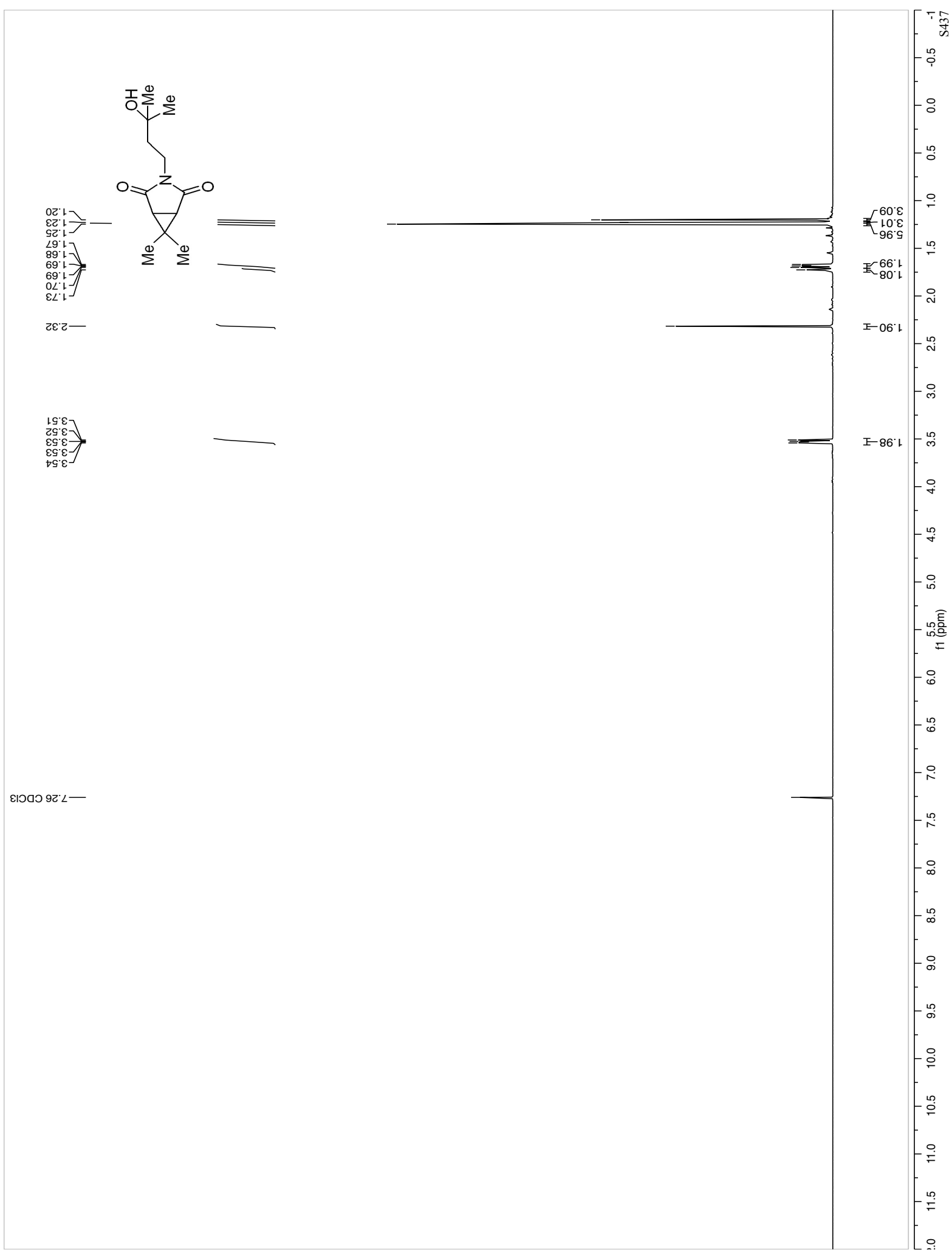
— 77.2 CDCl₃

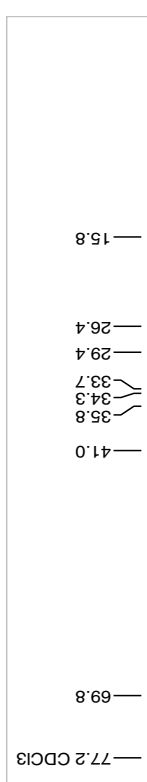
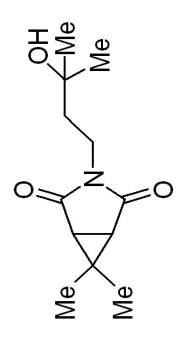
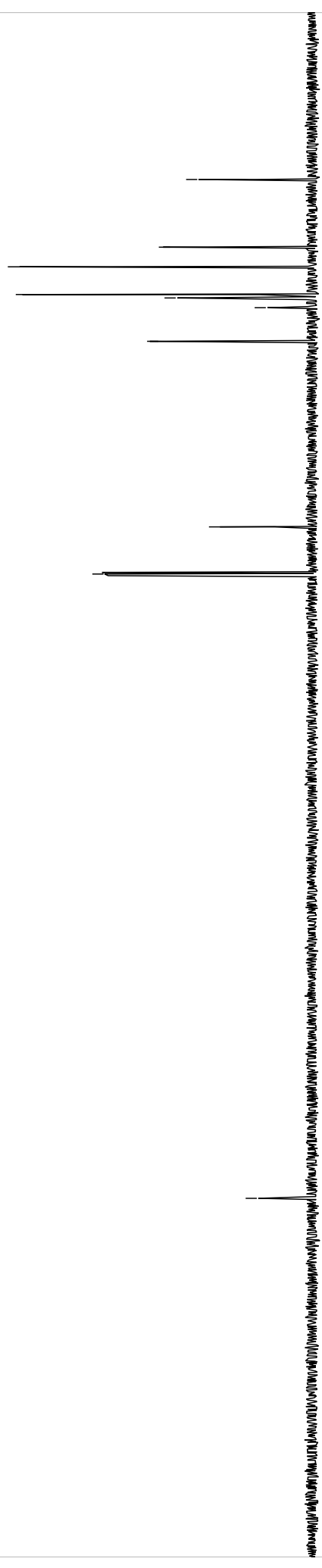




Parameter		Value
1	Origin	Varian
2	Spectrometer	inova
3	Solvent	CDCl3
4	Temperature	20.0
5	Pulse Sequence	s2pul
6	Experiment	1D
7	Probe	QUAD
8	Number of Scans	8
9	Receiver Gain	46
10	Relaxation Delay	0.0000
11	Pulse Width	0.0000
12	Acquisition Time	4.6645
13	Spectrometer Frequency	499.69
14	Spectral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

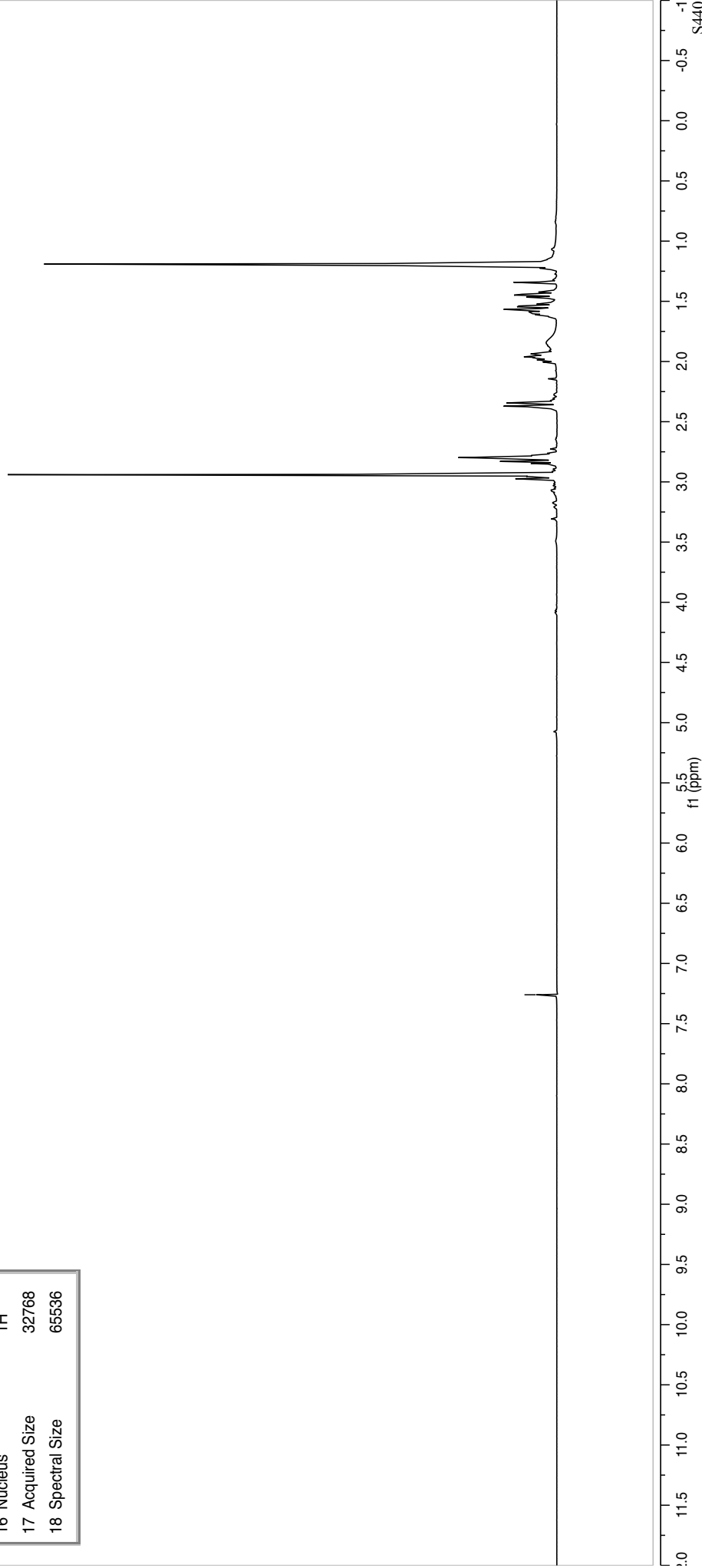
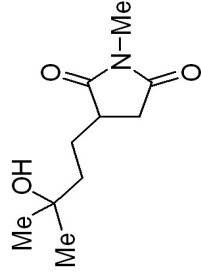




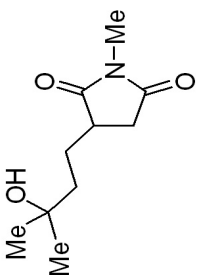


7.3 CDCl3

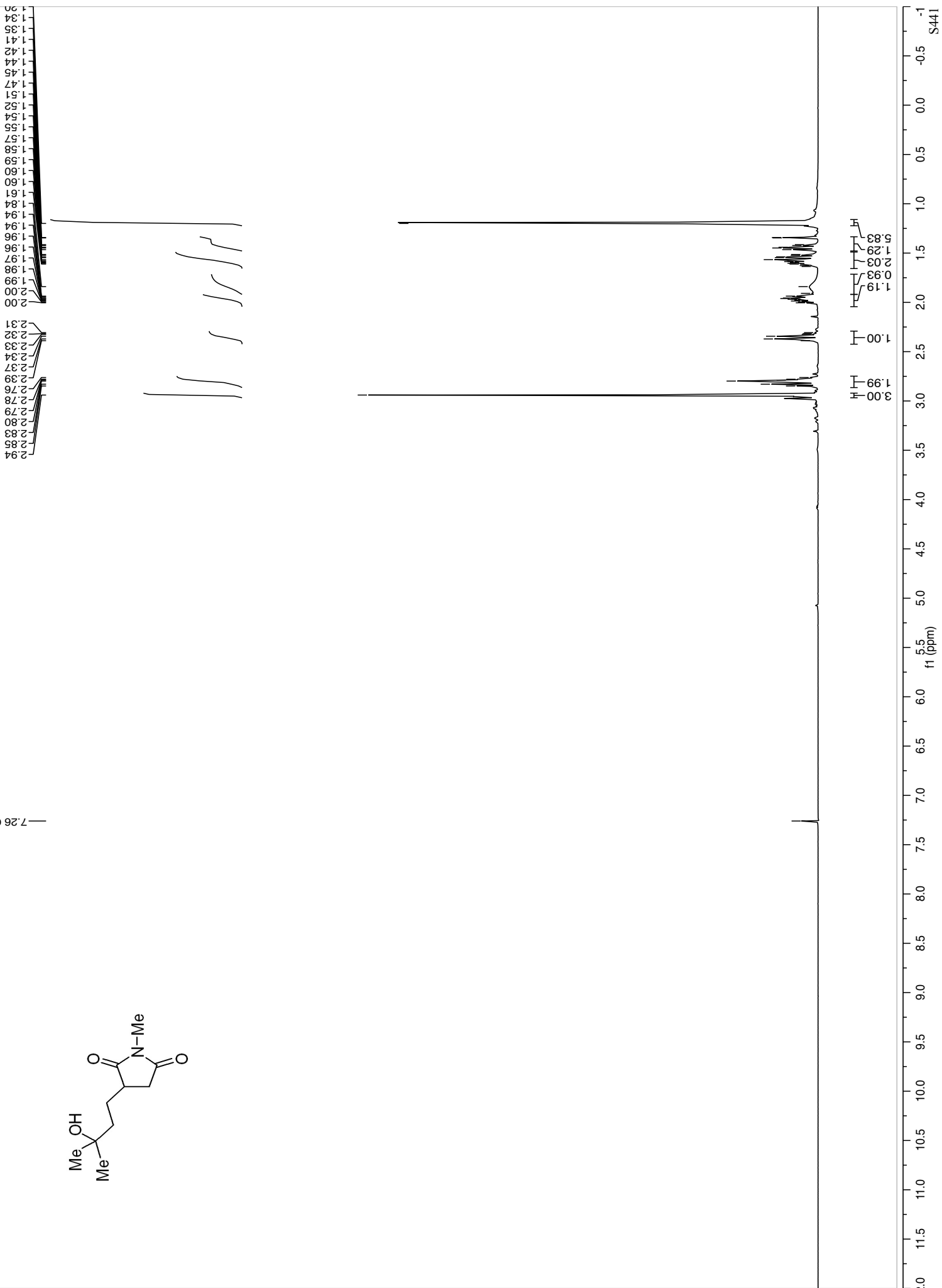
Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	8
9 Receiver Gain	36
10 Relaxation Delay	0.0000
11 Pulse Width	0.0000
12 Acquisition Time	4.6645
13 Spectrometer Frequency	499.69
14 Spectral Width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



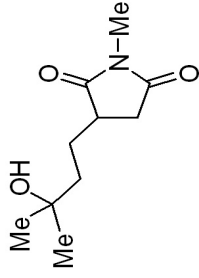
S440



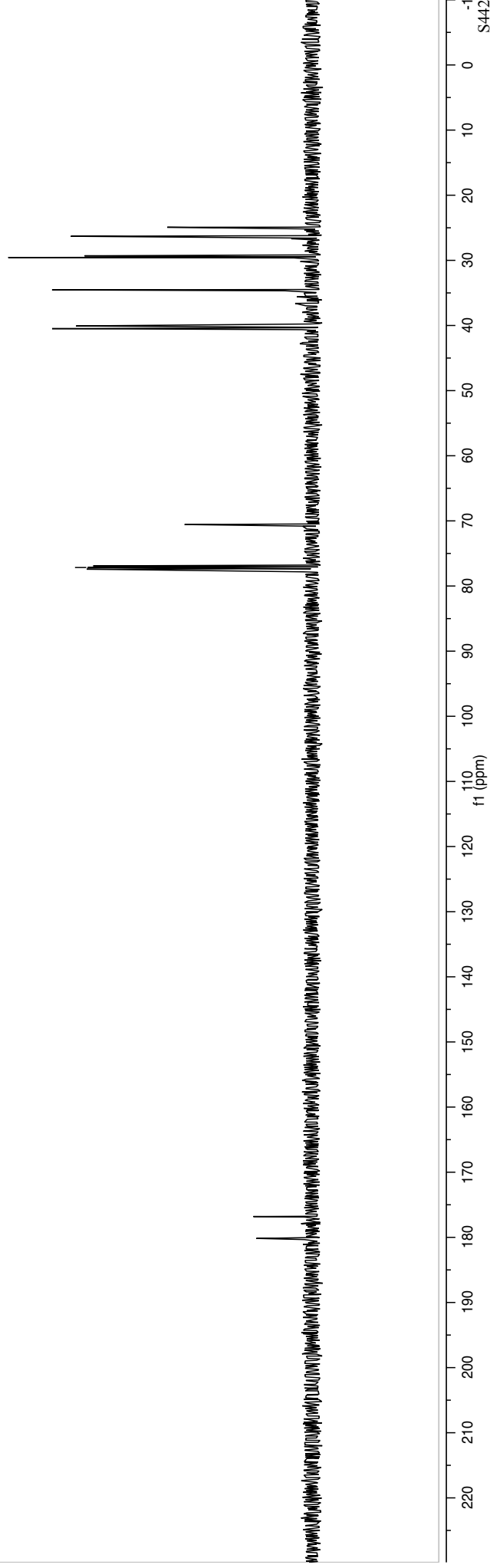
7.26 CDCl₃

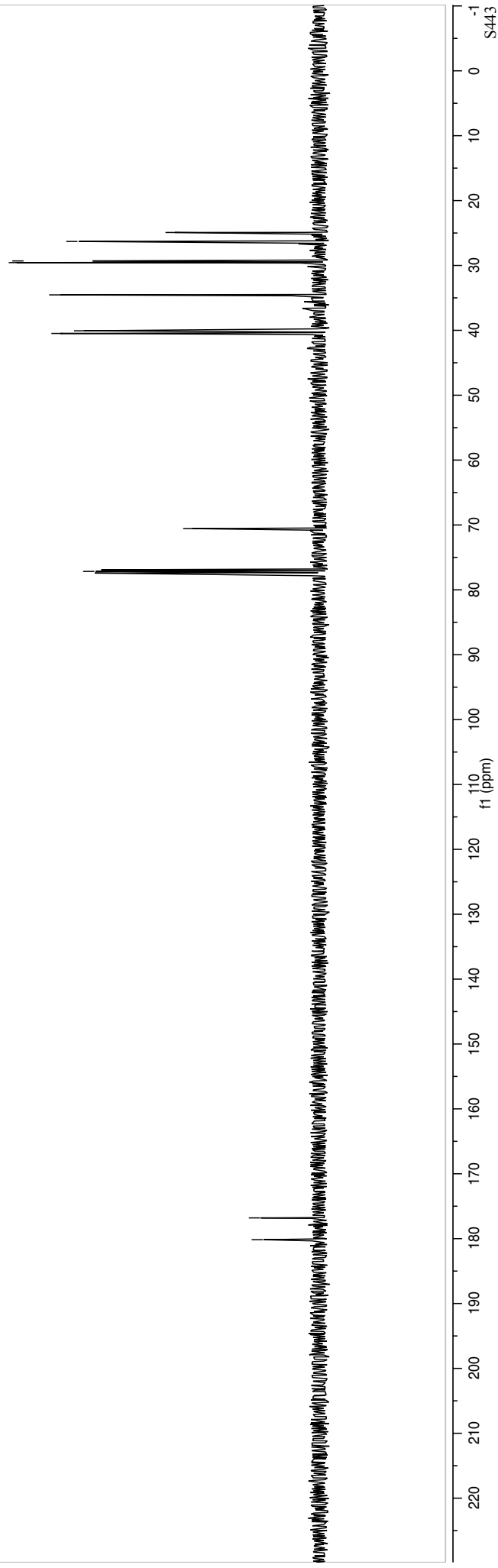
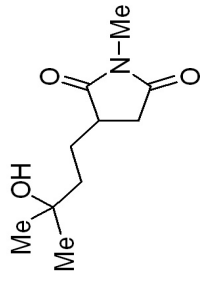


77.2 CDCl3

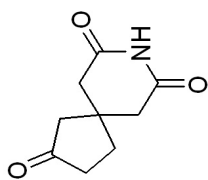


Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	112
9 Receiver Gain	60
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.0863
13 Spectrometer Frequency	125.66
14 Spectral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

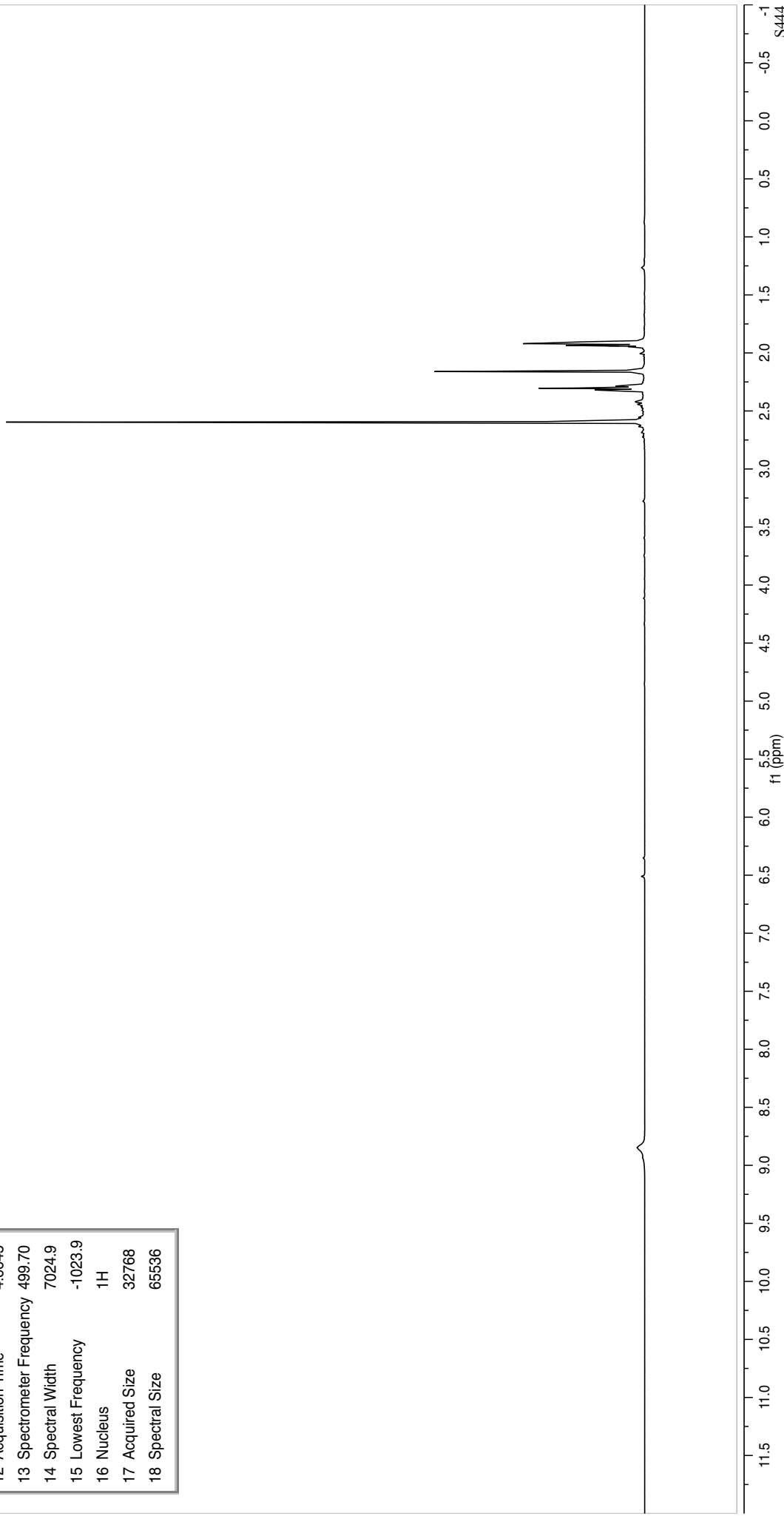


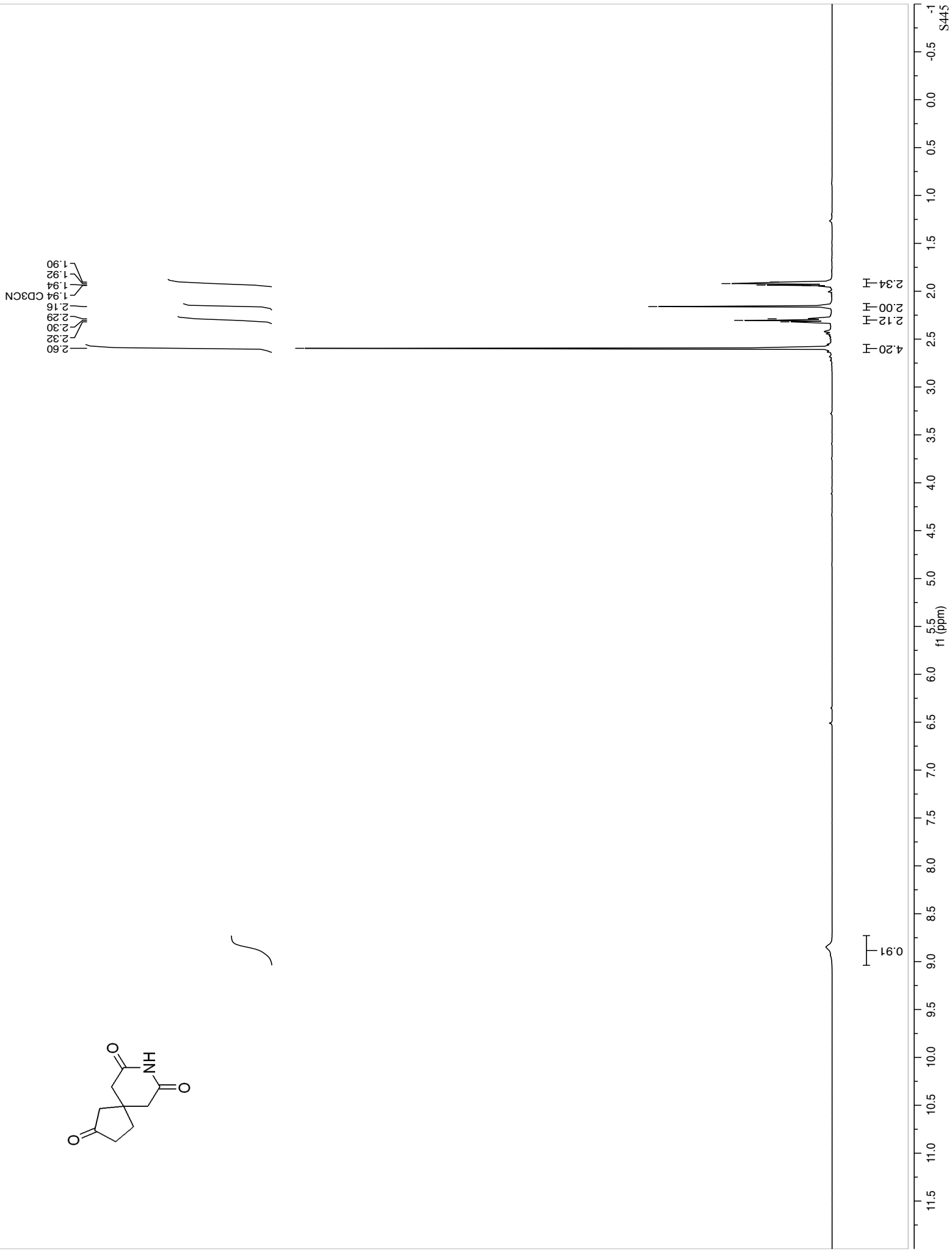
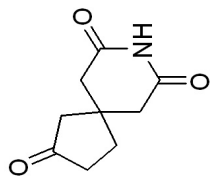


Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CD3CN
4 Temperature	29.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	8
9 Receiver Gain	41
10 Relaxation Delay	0.0000
11 Pulse Width	0.0000
12 Acquisition Time	4.6645
13 Spectrometer Frequency	499.70
14 Spectral Width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

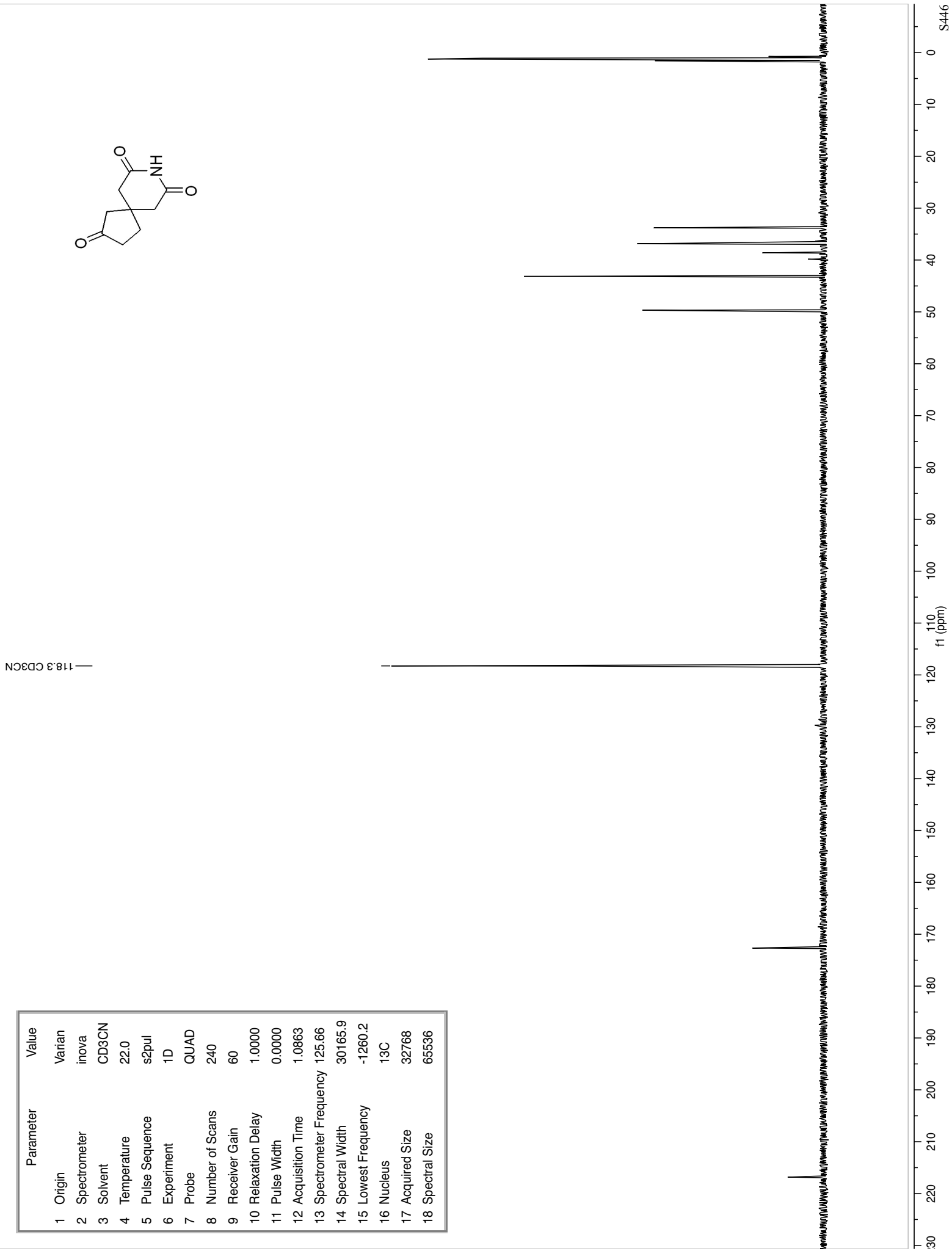
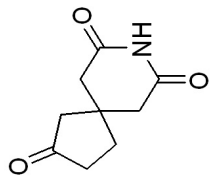


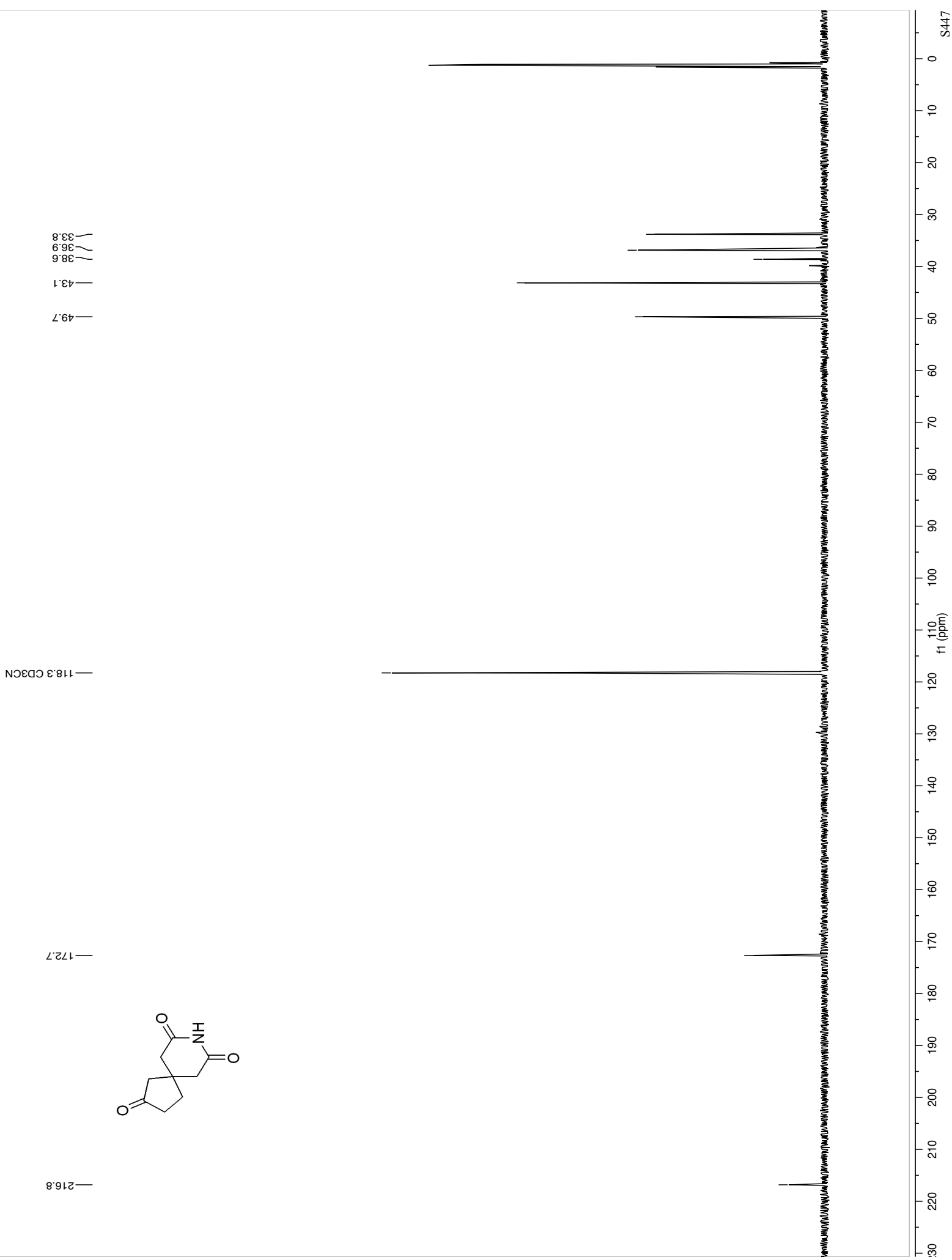
— 1.94 CD3CN



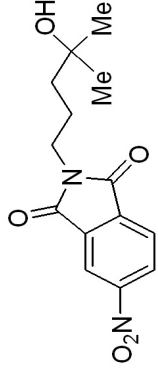


Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CD3CN
4 Temperature	22.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	240
9 Receiver Gain	60
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.0863
13 Spectrometer Frequency	125.66
14 Spectral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

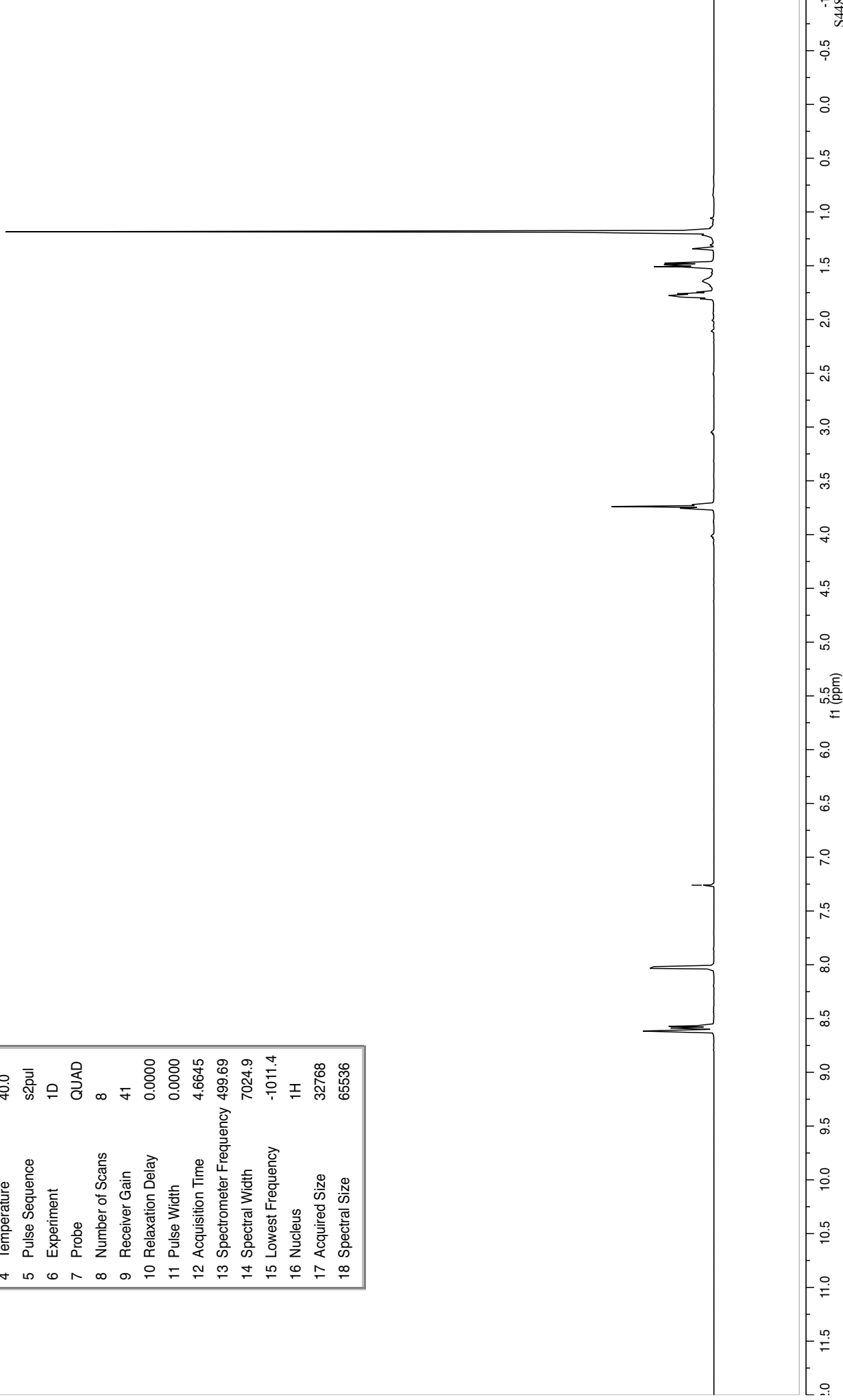


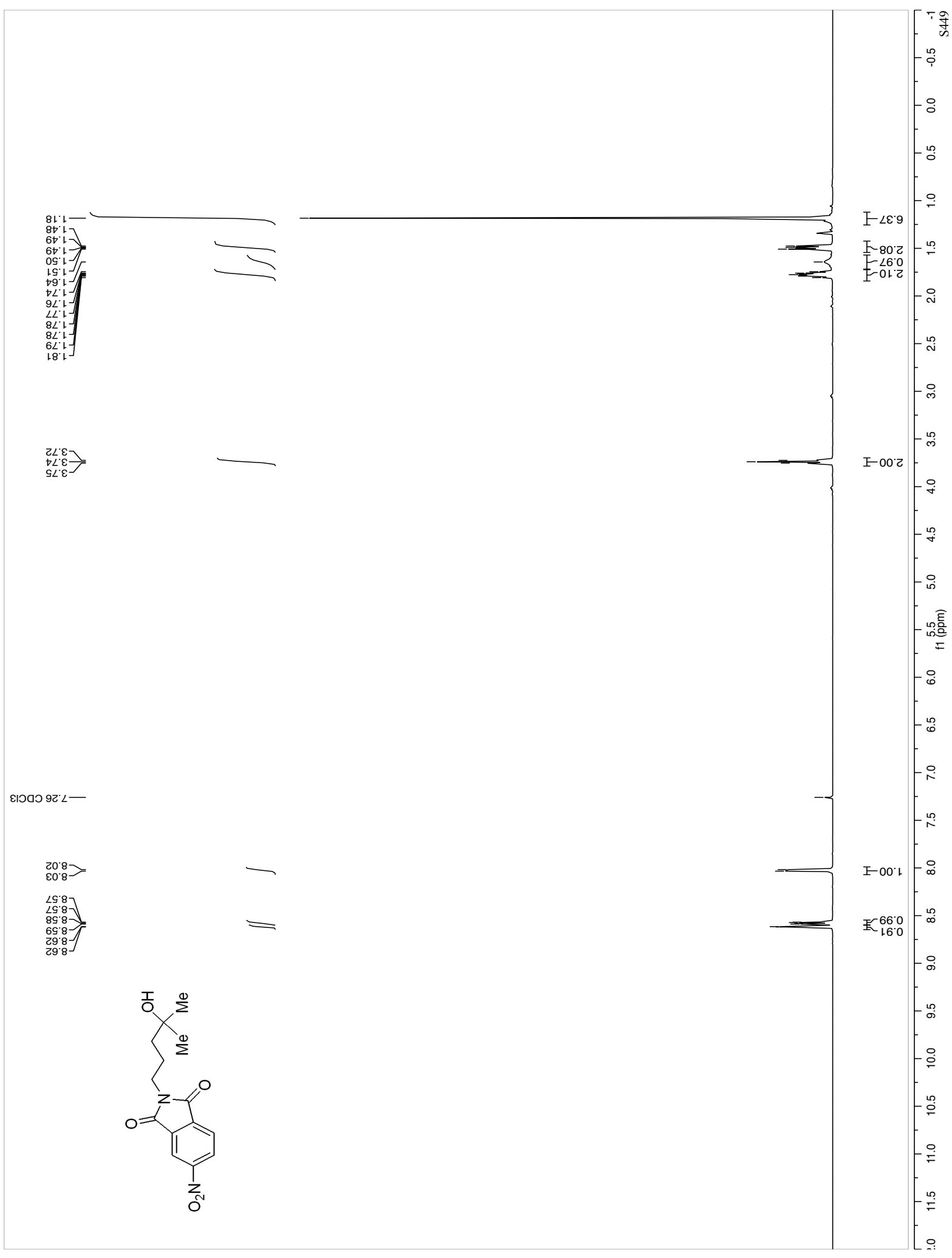
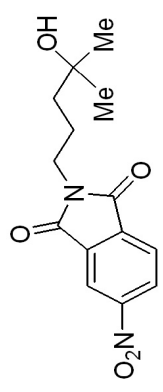


7.26 CDCl₃

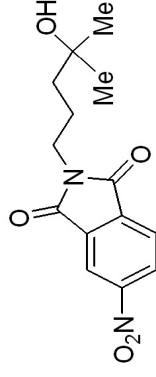


Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl ₃
4 Temperature	40.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	8
9 Receiver Gain	41
10 Relaxation Delay	0.0000
11 Pulse Width	0.0000
12 Acquisition Time	4.6645
13 Spectrometer Frequency	499.69
14 Spectral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

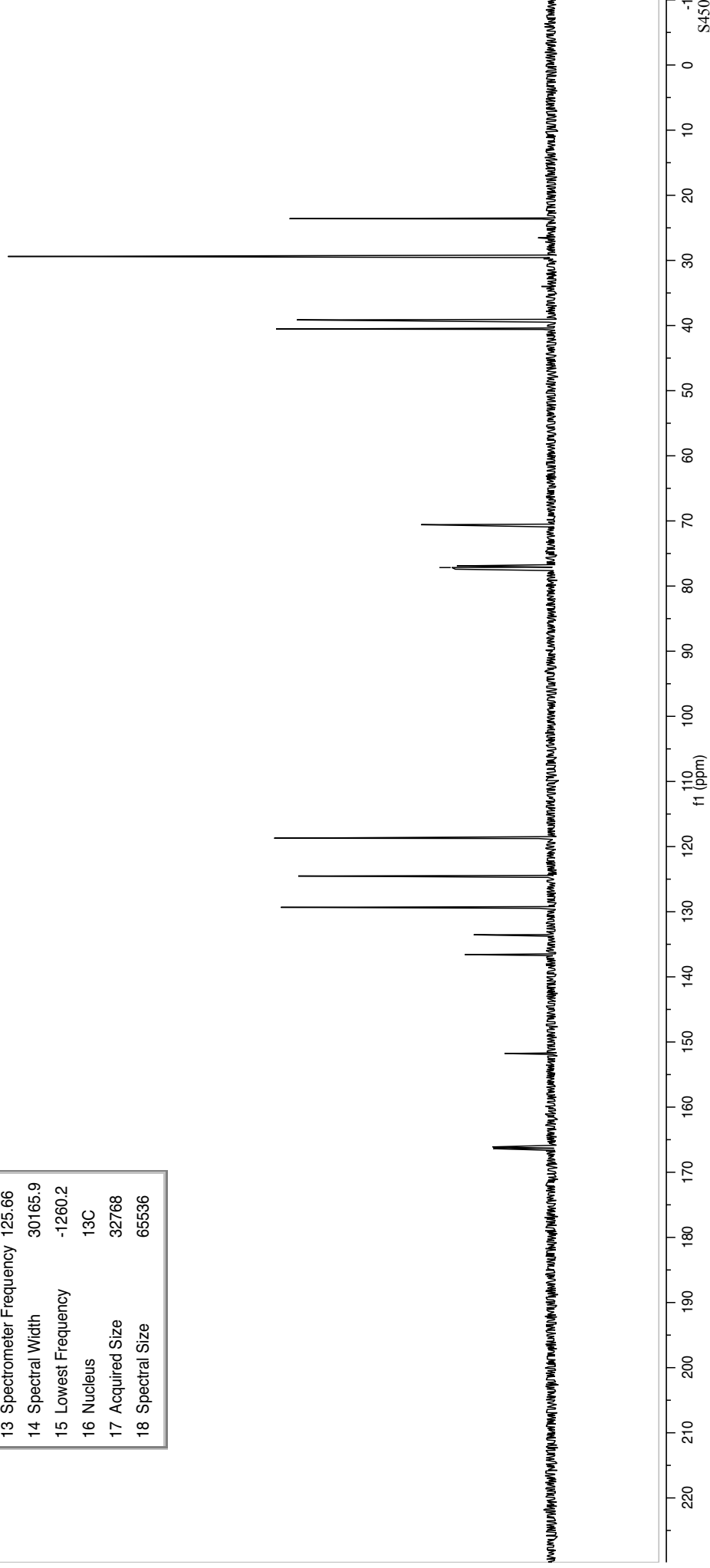


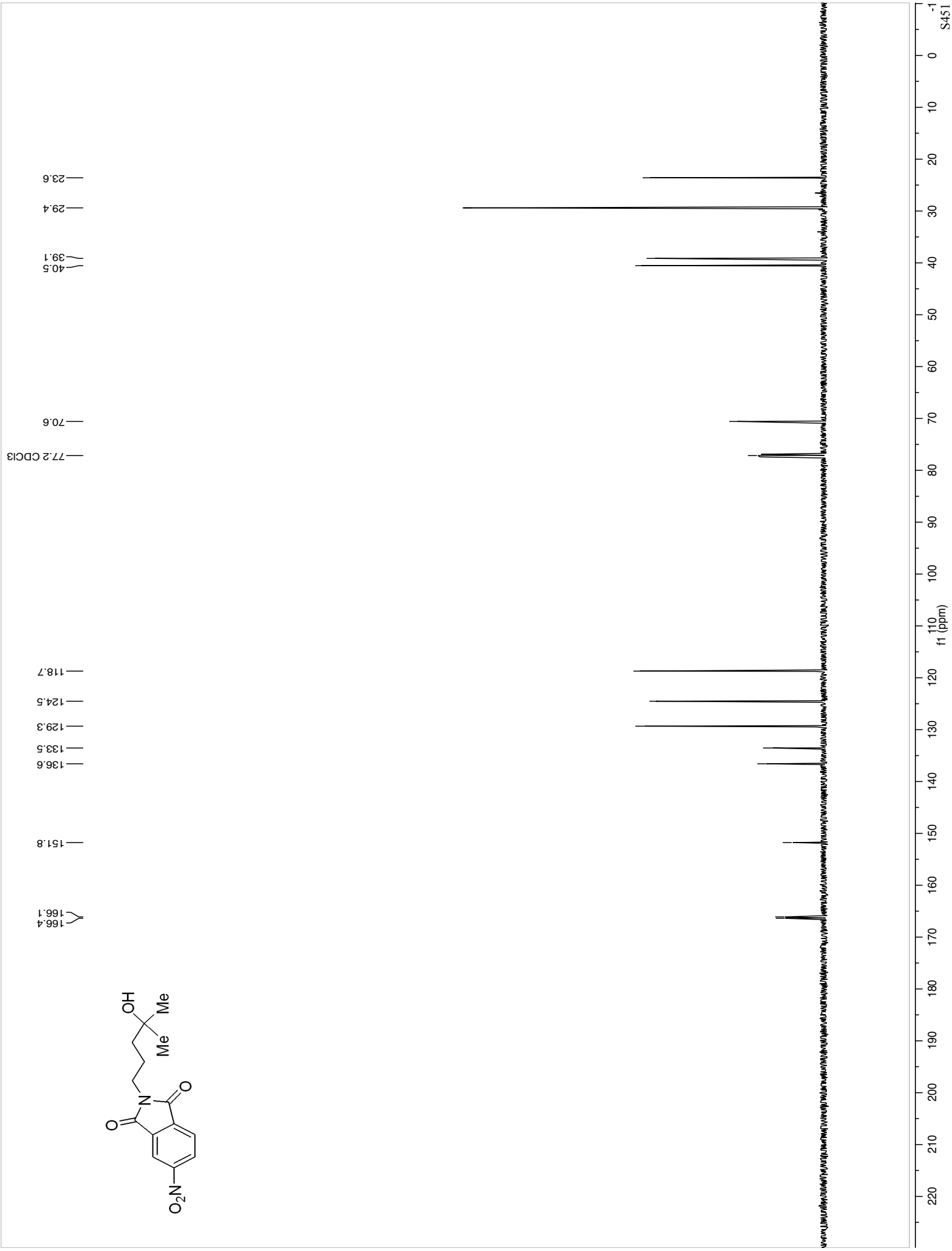
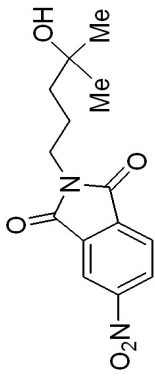


Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	40.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	64
9 Receiver Gain	60
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.0863
13 Spectrometer Frequency	125.66
14 Spectral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

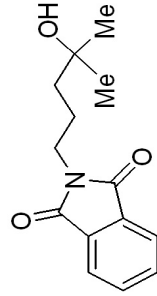


— 77.16 CDCl3

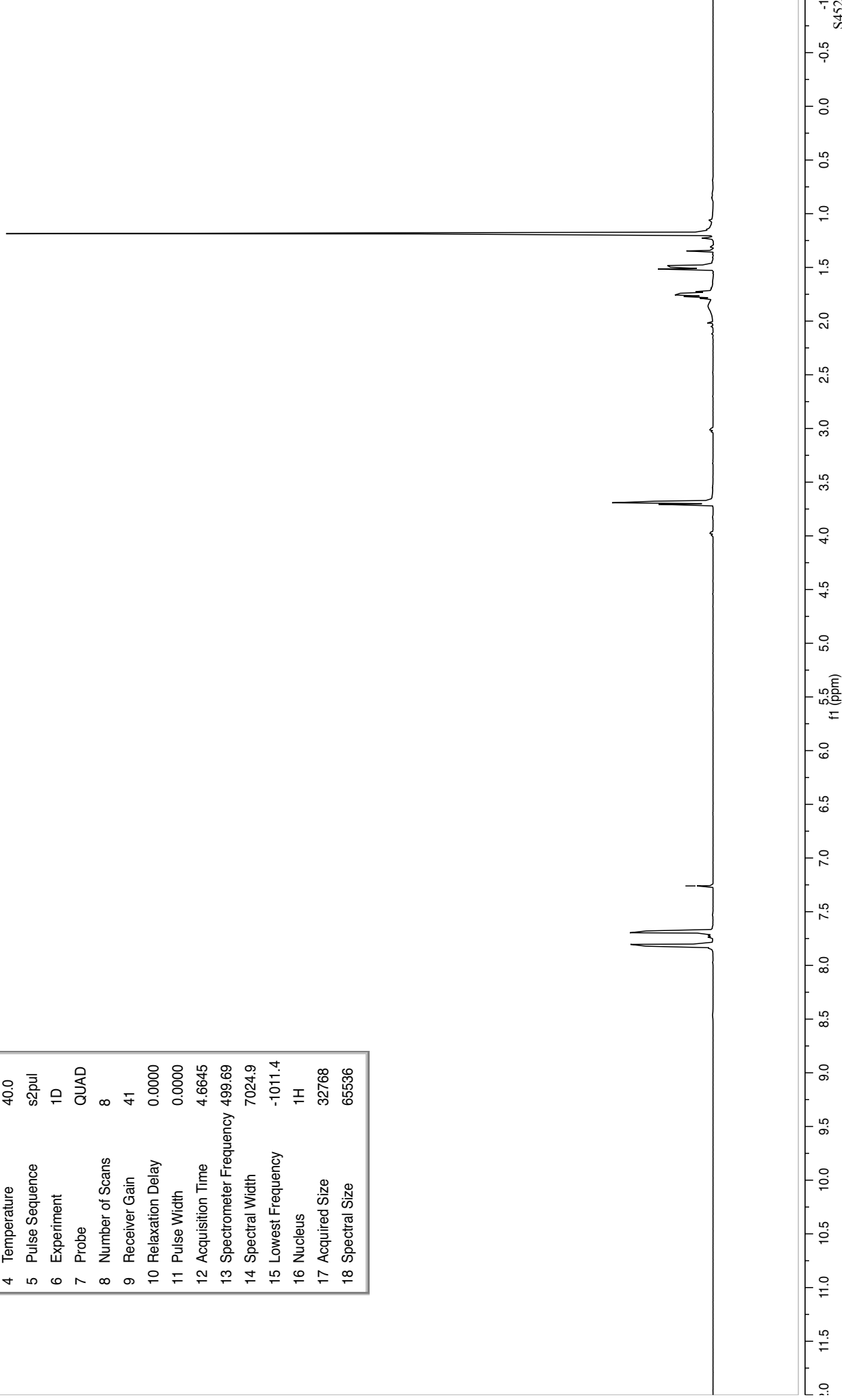


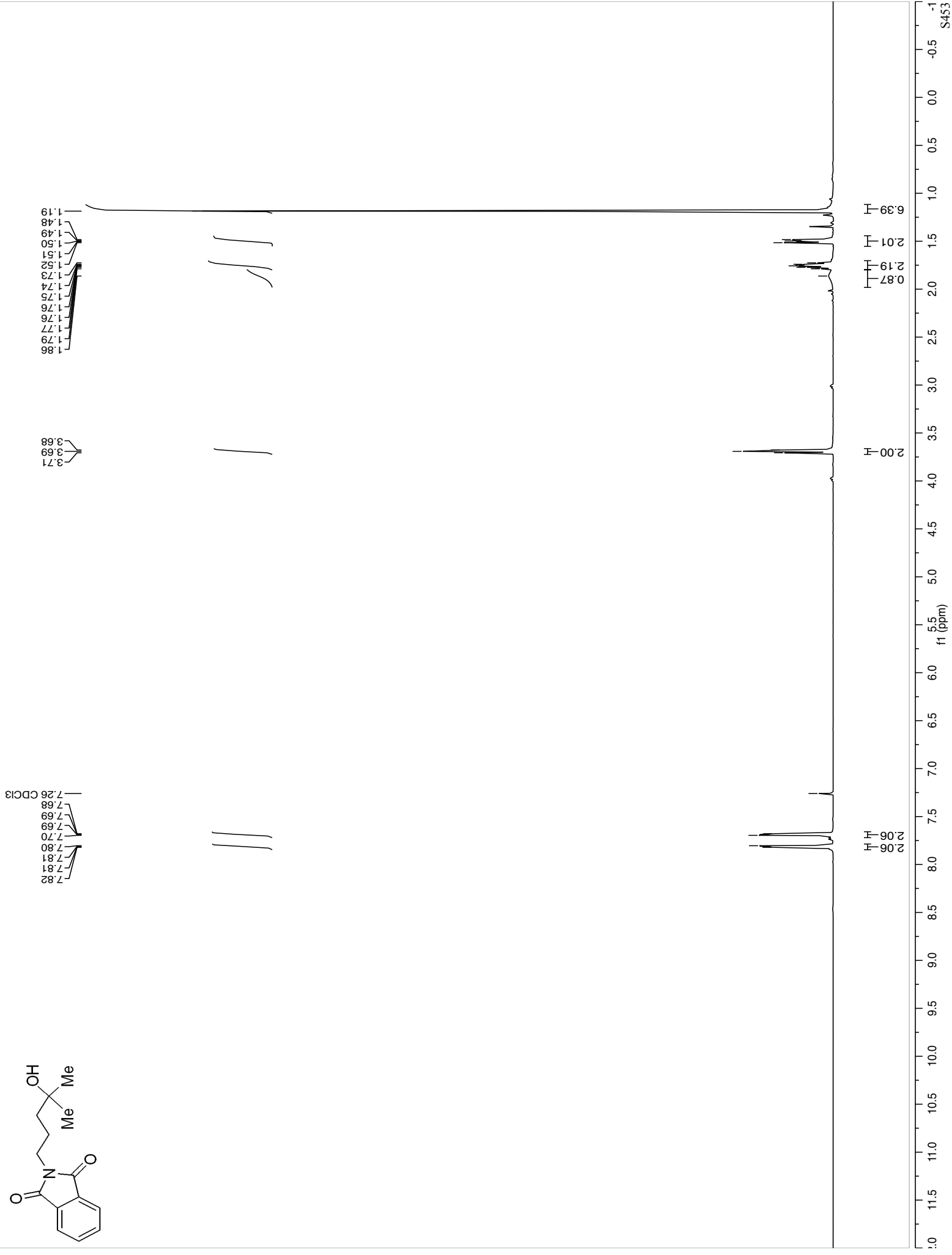
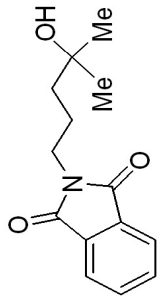


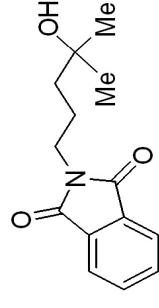
— 7.26 CDCl₃



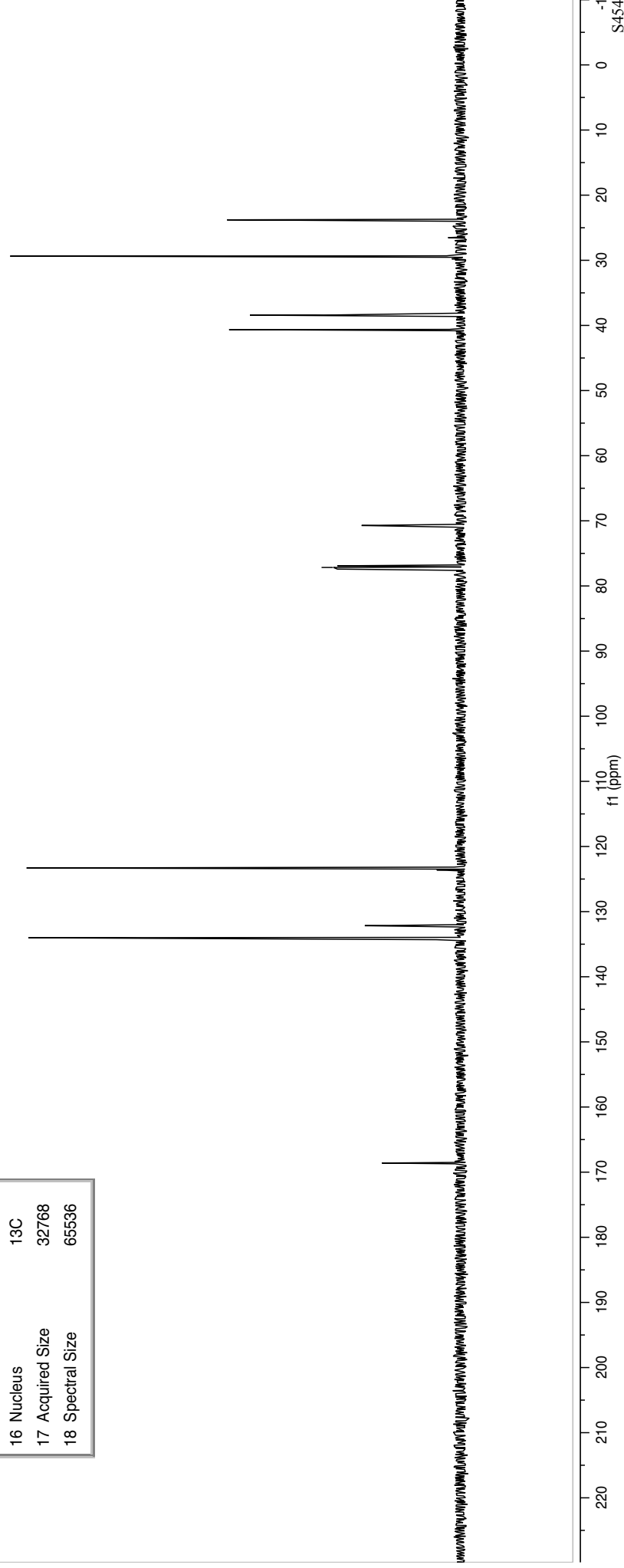
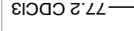
Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl ₃
4 Temperature	40.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	8
9 Receiver Gain	41
10 Relaxation Delay	0.0000
11 Pulse Width	0.0000
12 Acquisition Time	4.6645
13 Spectrometer Frequency	499.69
14 Spectral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

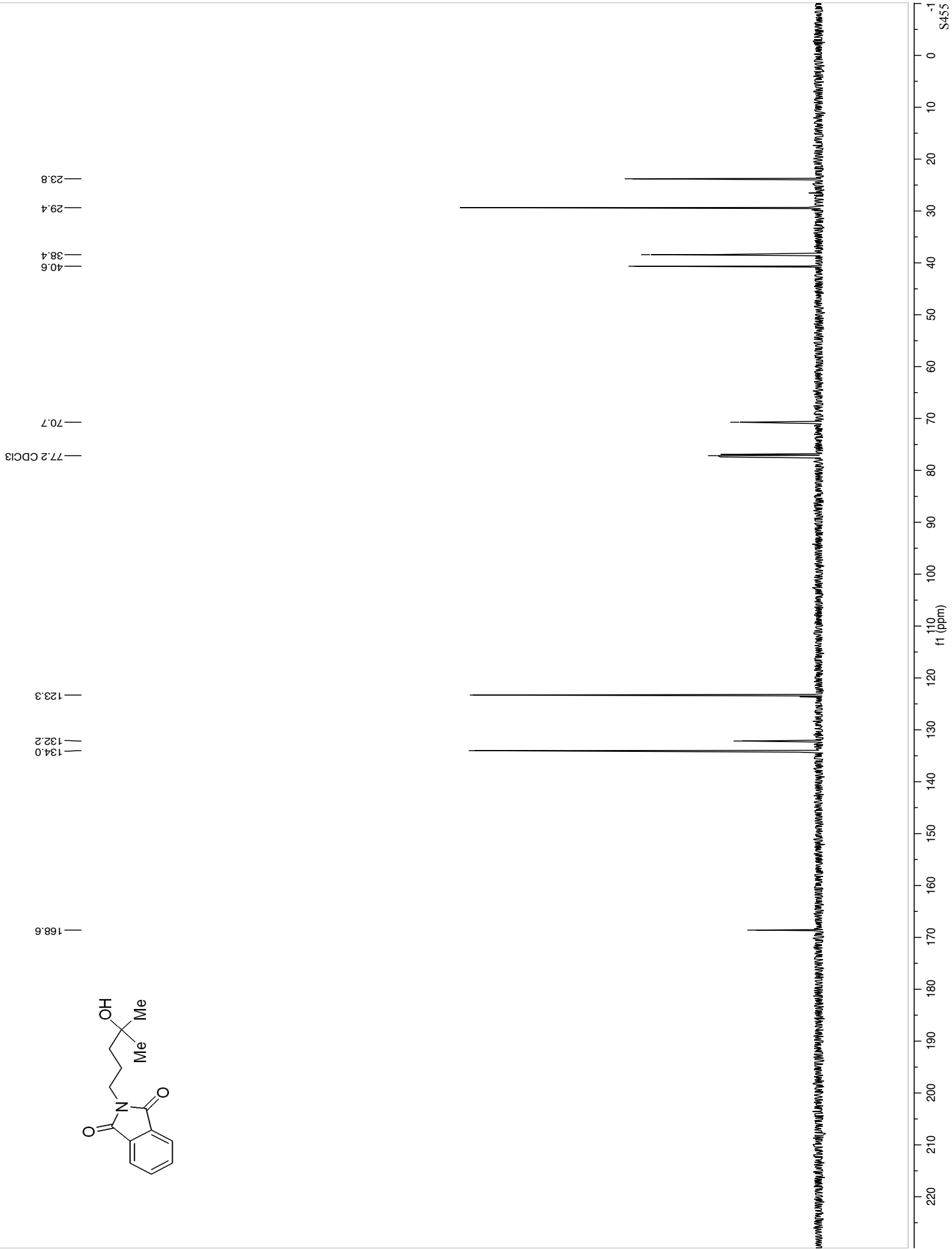
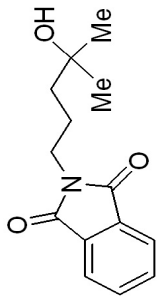




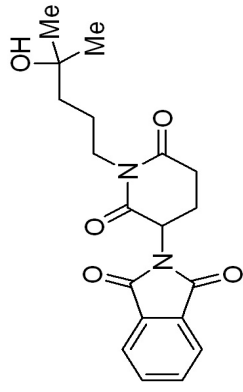


Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCI3
4 Temperature	40.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QPAD
8 Number of Scans	64
9 Receiver Gain	60
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.0863
13 Spectrometer Frequency	125.66
14 Spectral Width	30165.9
15 Lowest Frequency	-1260.2
16 Nucleus	13C
17 Acquired Size	32768
18 Spectral Size	65536

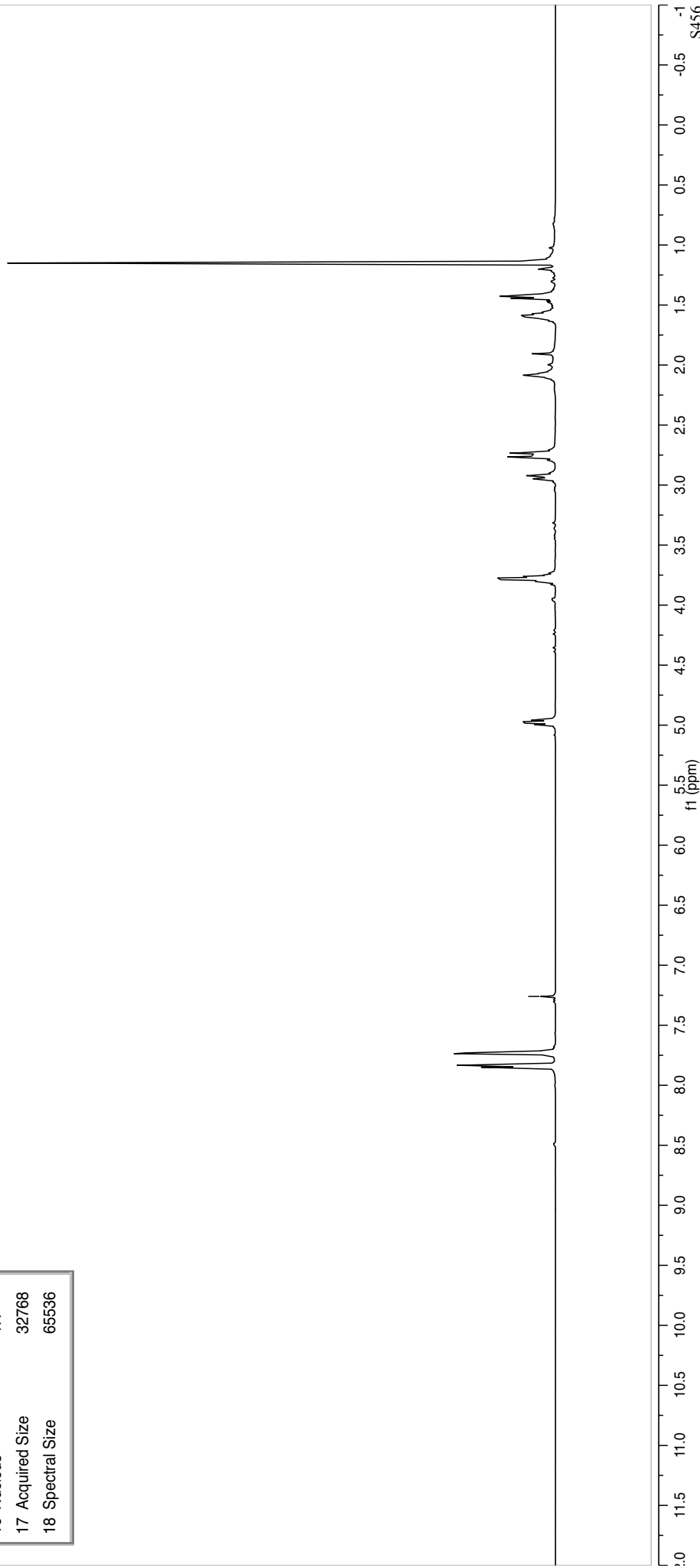




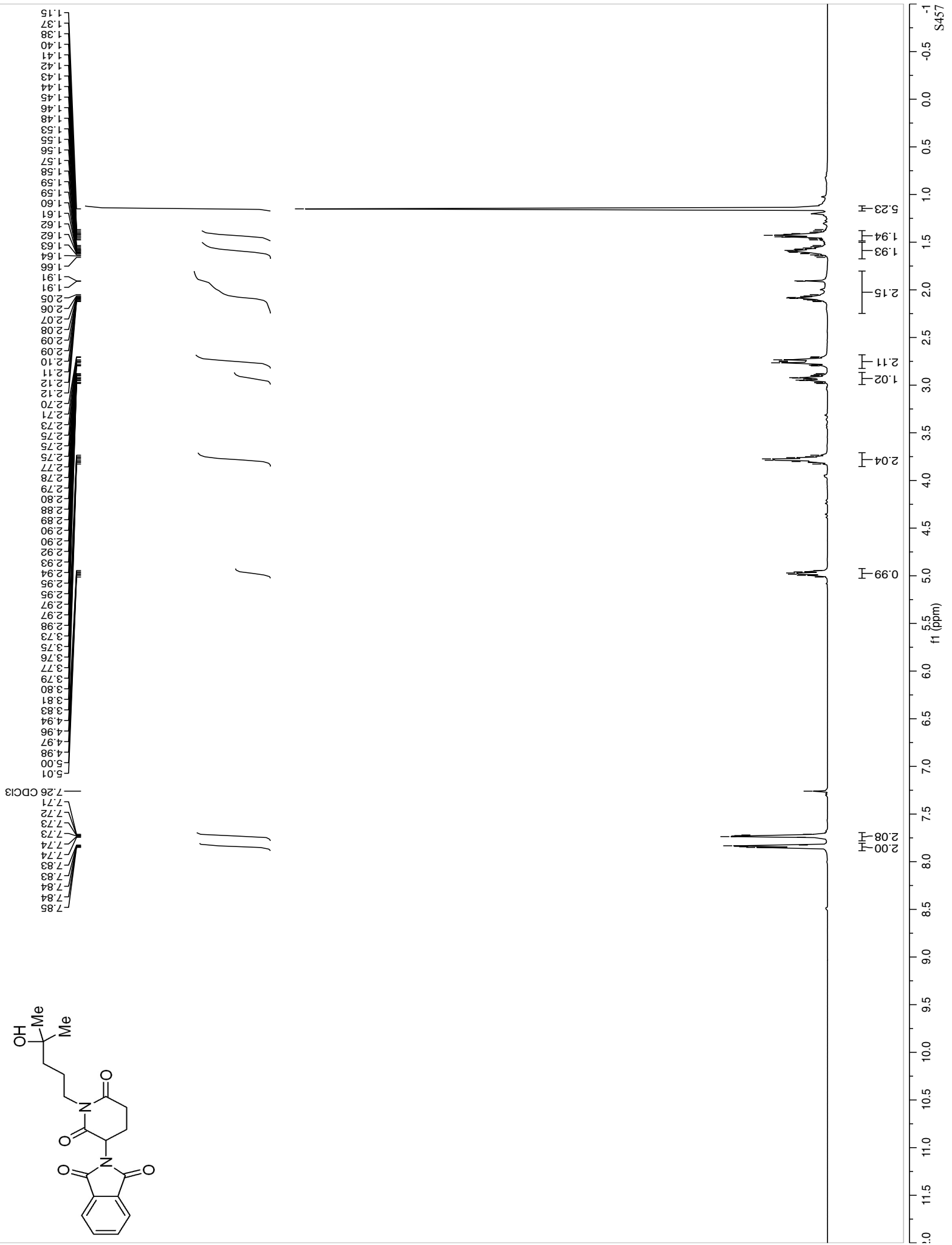
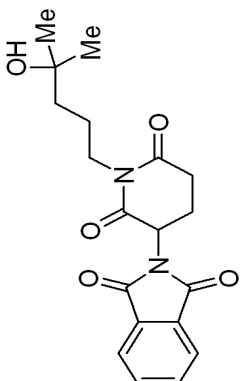
7.3 CDCl3



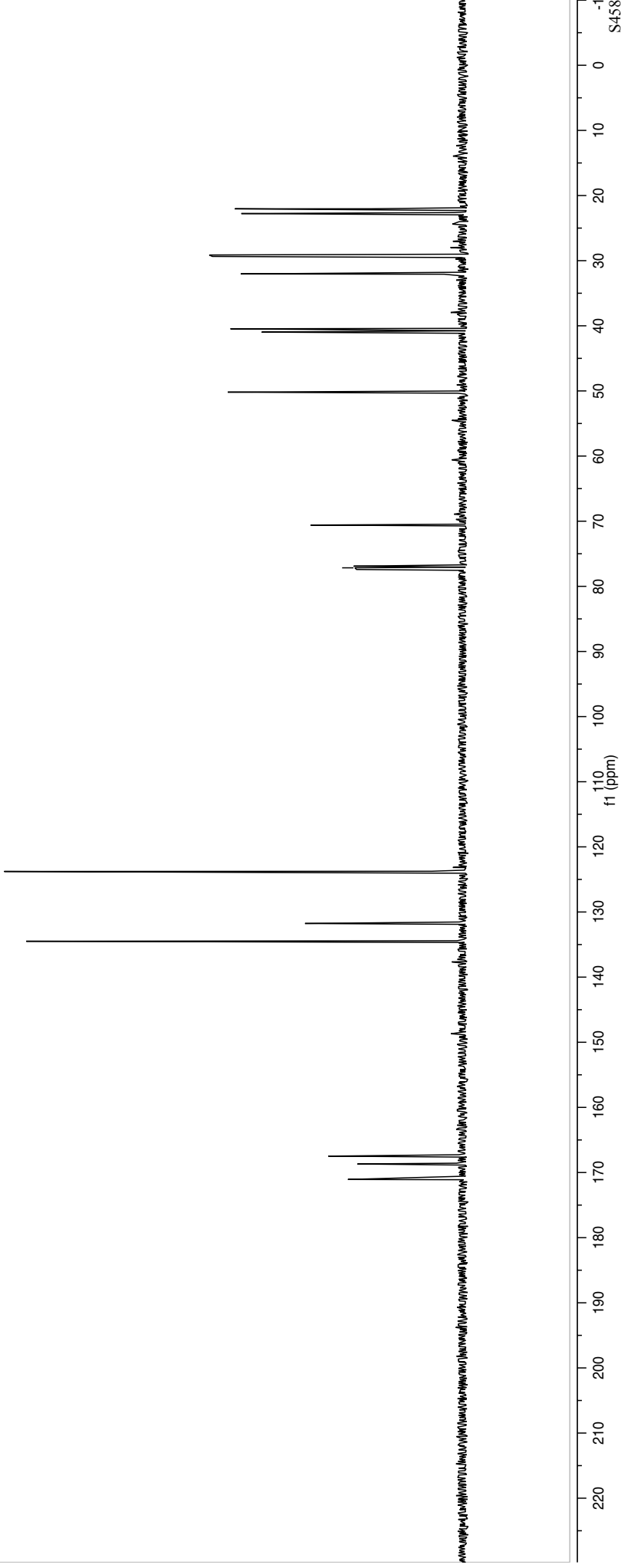
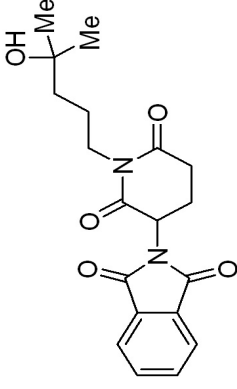
Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	8
9 Receiver Gain	41
10 Relaxation Delay	0.0000
11 Pulse Width	0.0000
12 Acquisition Time	4.6645
13 Spectrometer Frequency	499.69
14 Spectral Width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



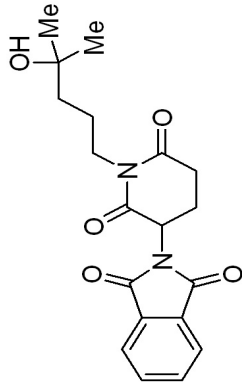
S456

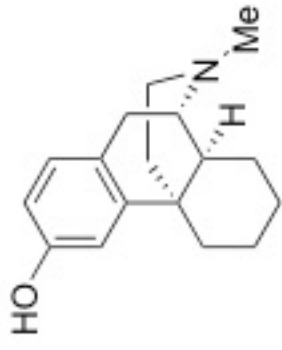


Parameter		Value
1	Origin	Varian
2	Spectrometer	inova
3	Solvent	CDCl3
4	Temperature	20.0
5	Pulse Sequence	s2pul
6	Experiment	1D
7	Probe	QUAD
8	Number of Scans	112
9	Receiver Gain	60
10	Relaxation Delay	1.0000
11	Pulse Width	0.0000
12	Acquisition Time	1.0863
13	Spectrometer Frequency	125.66
14	Spectral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

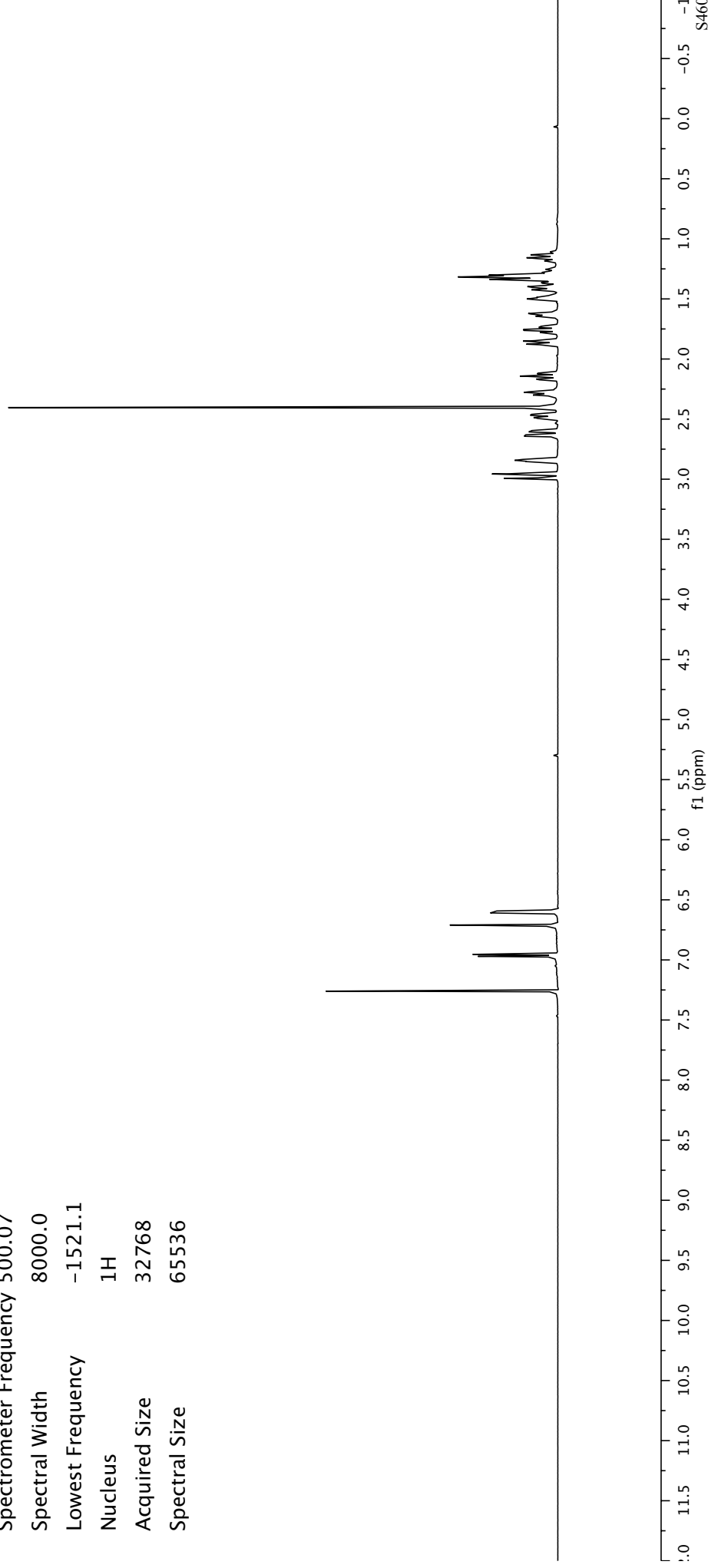


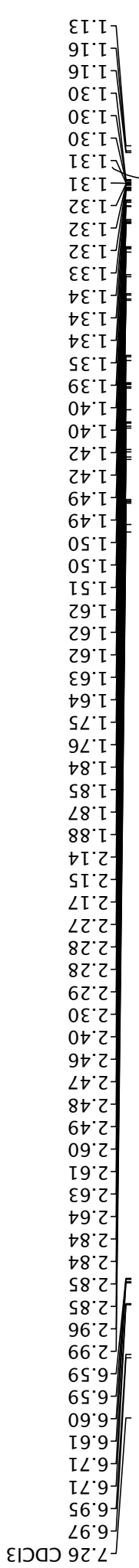
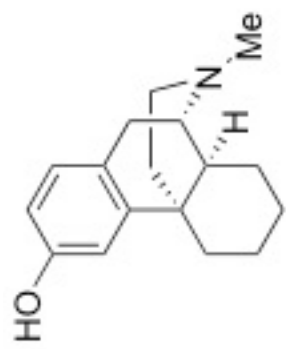
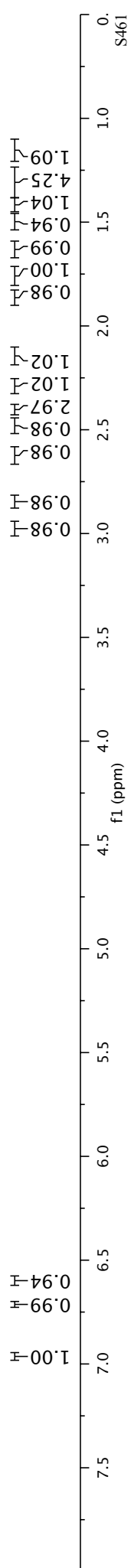
S458

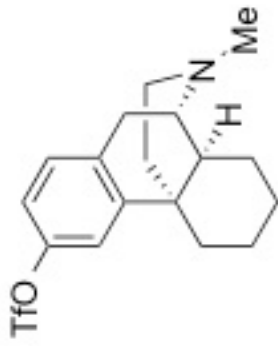




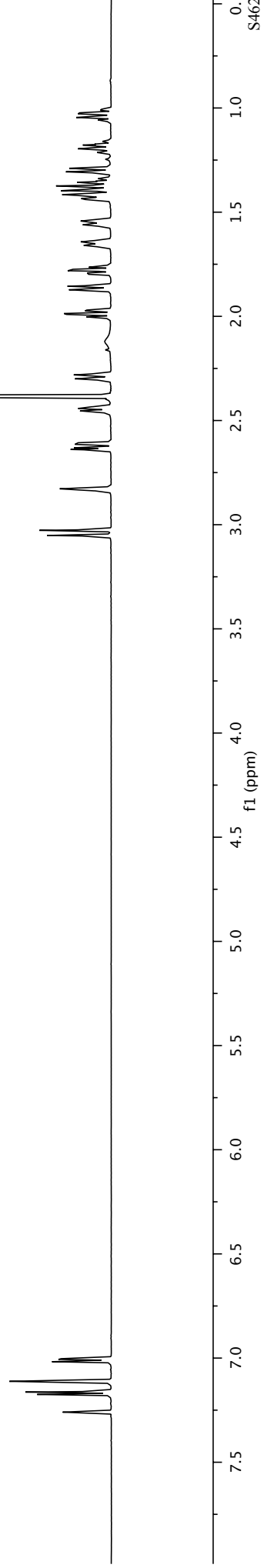
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	38
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1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

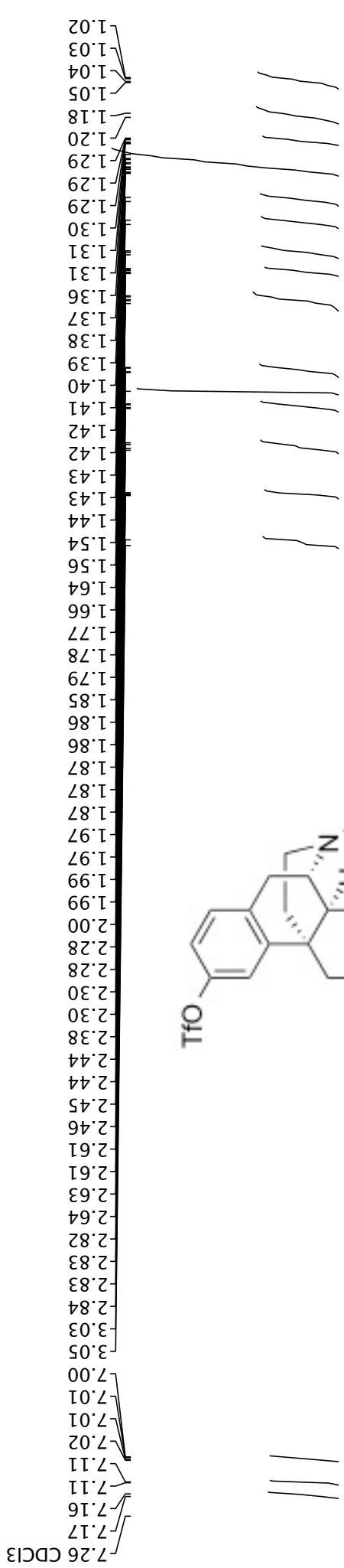
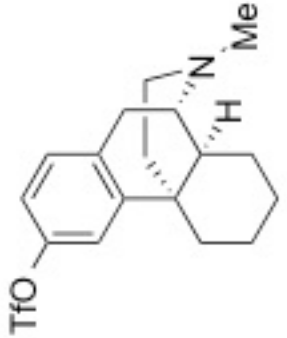
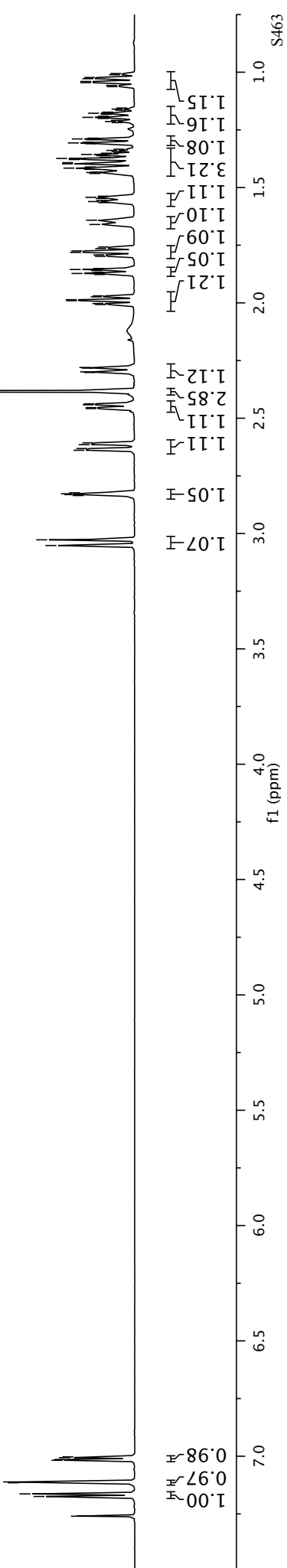


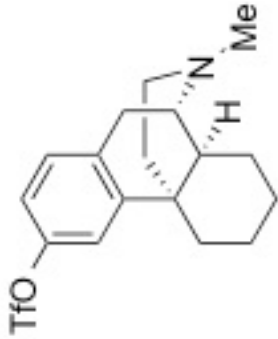




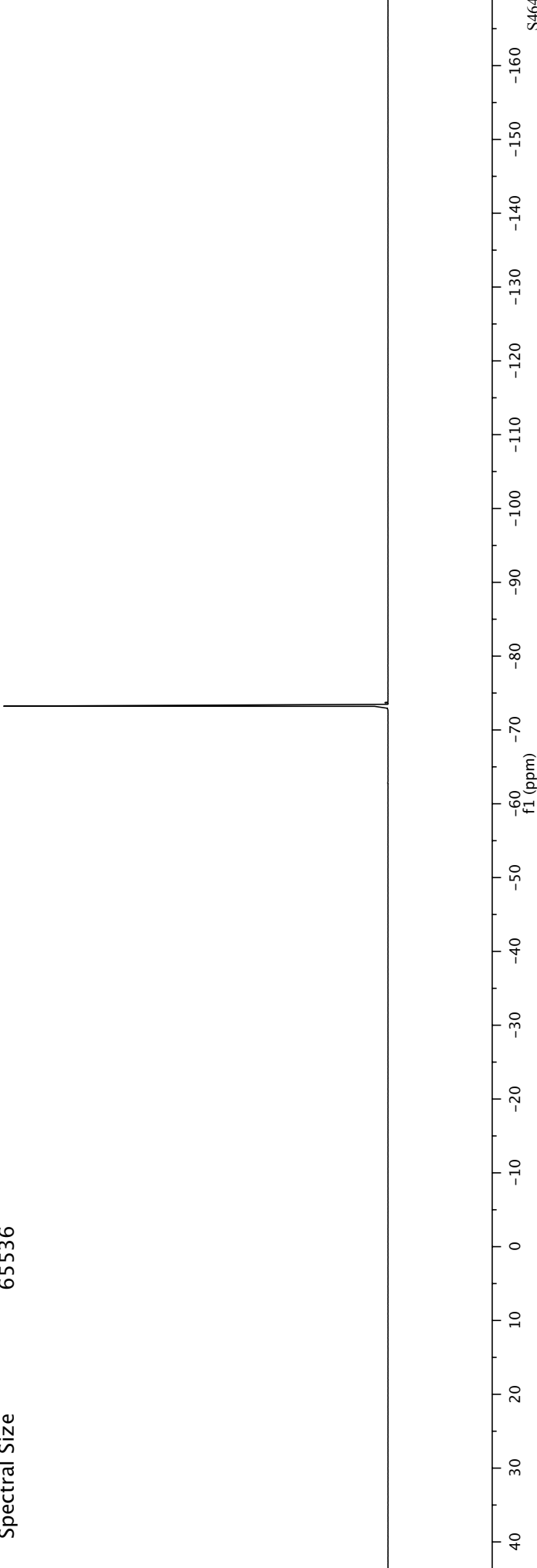
Parameter	Value
Origin	Varian
Spectrometer	vmrs
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	triax
Number of Scans	16
Receiver Gain	18
Relaxation Delay	15.0000
Pulse Width	0.0000
Acquisition Time	2.9098
Spectrometer Frequency	749.38
Spectral Width	5630.6
Lowest Frequency	355.3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

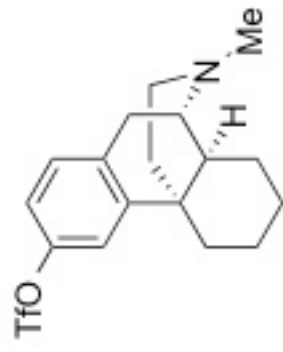




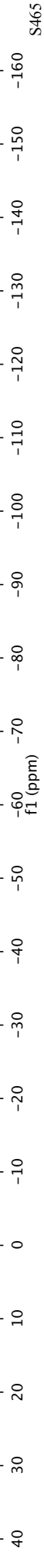


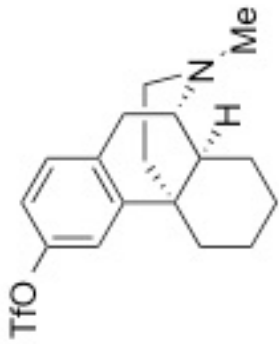
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	128
Receiver Gain	52
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency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



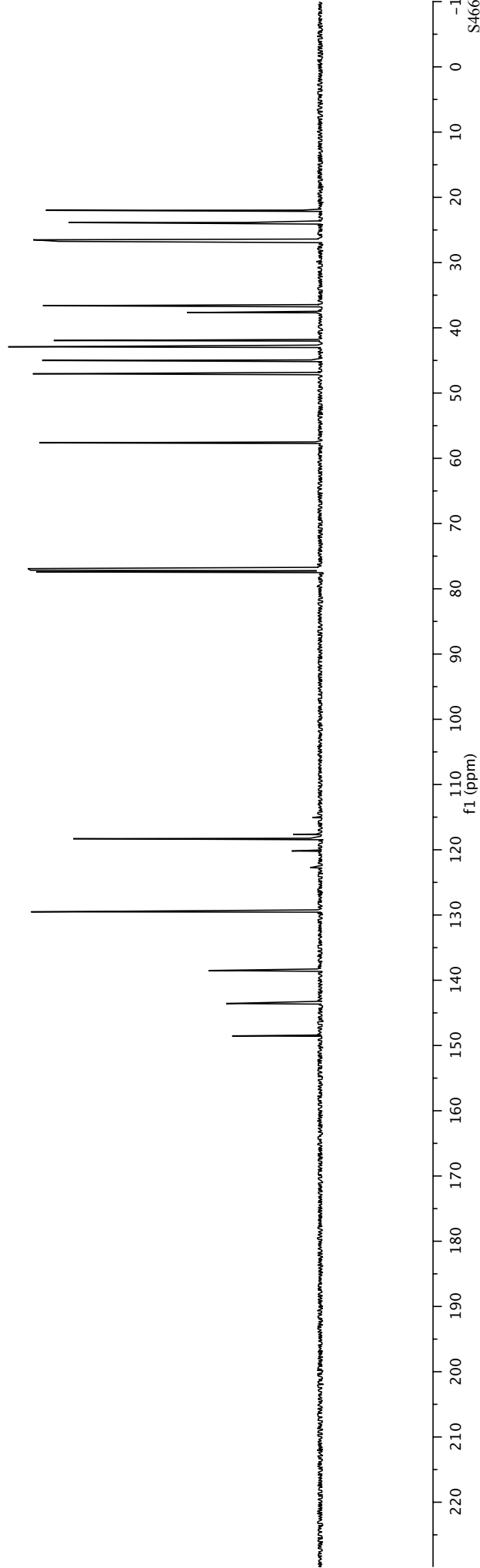


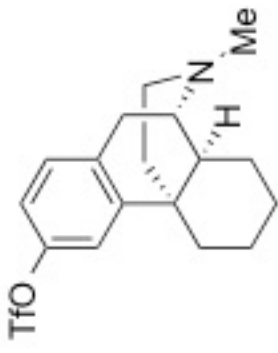
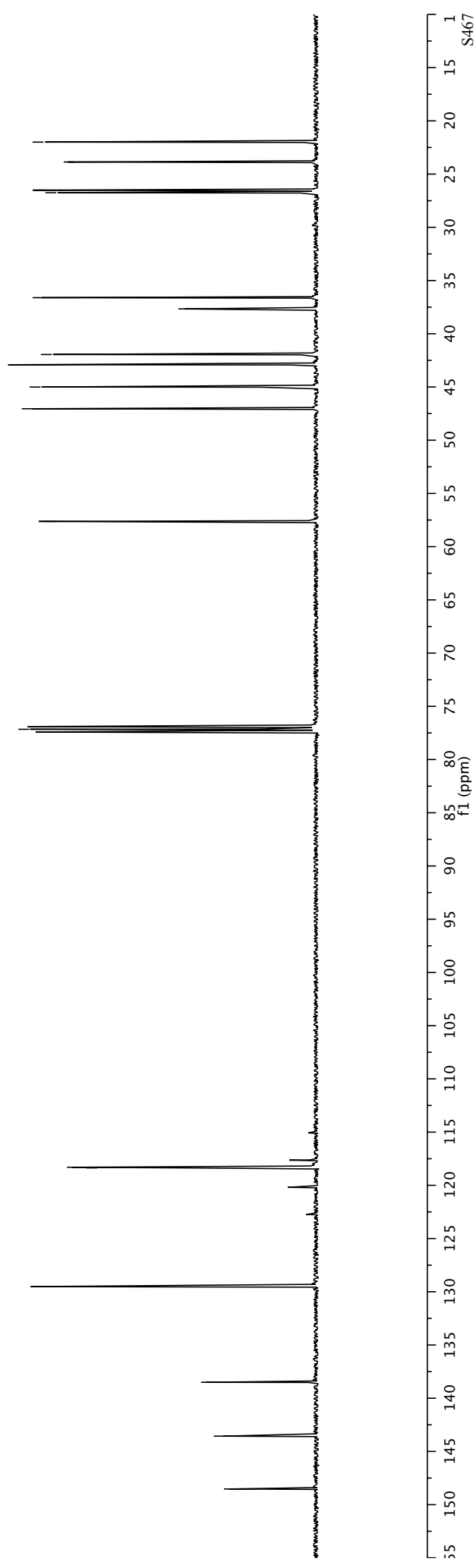
--73.22

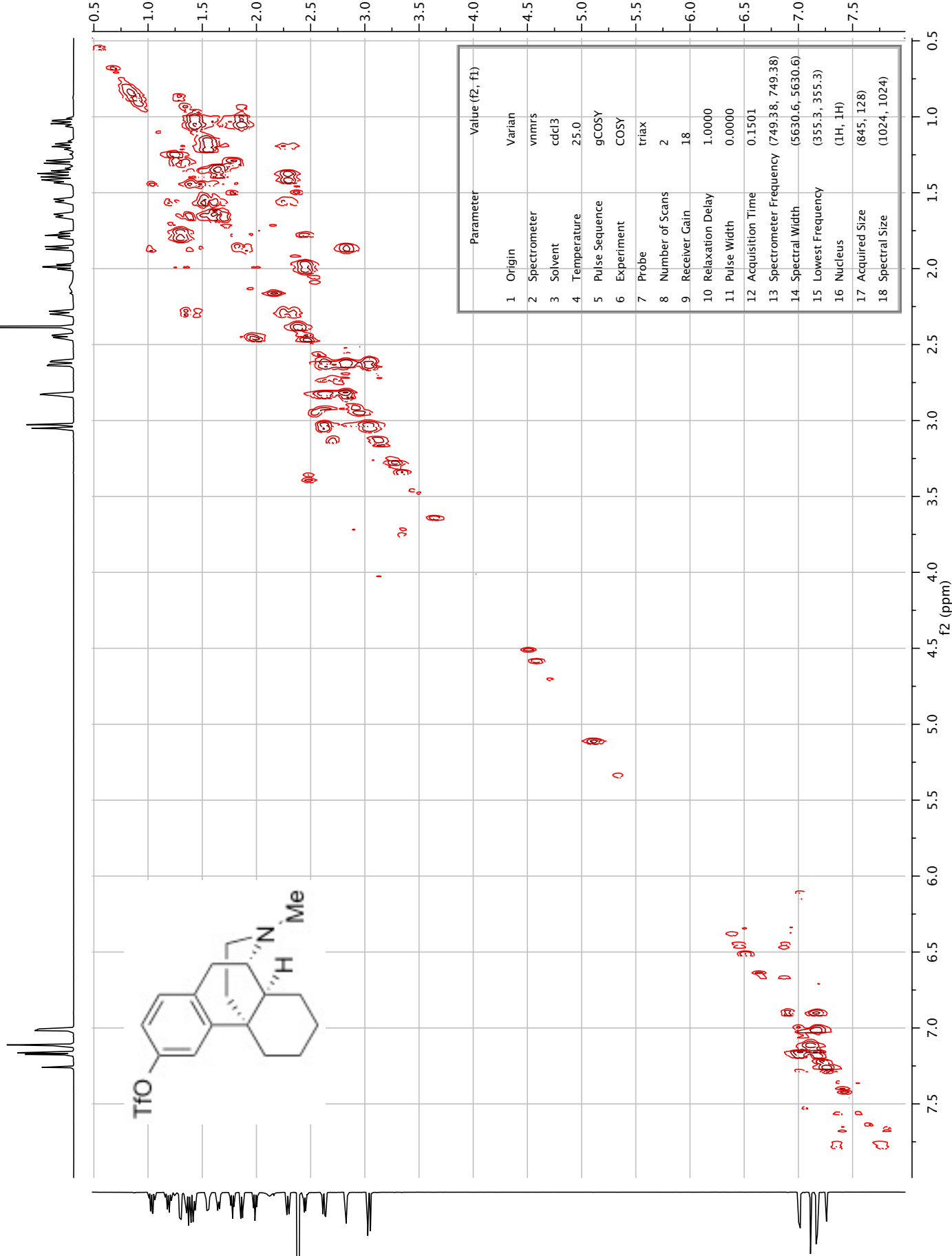
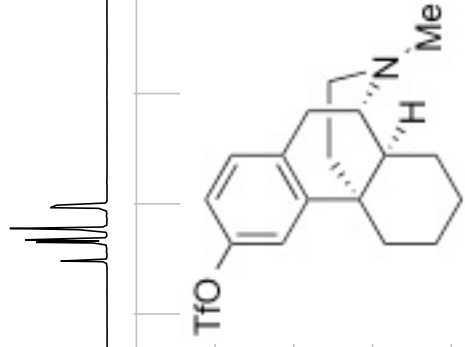




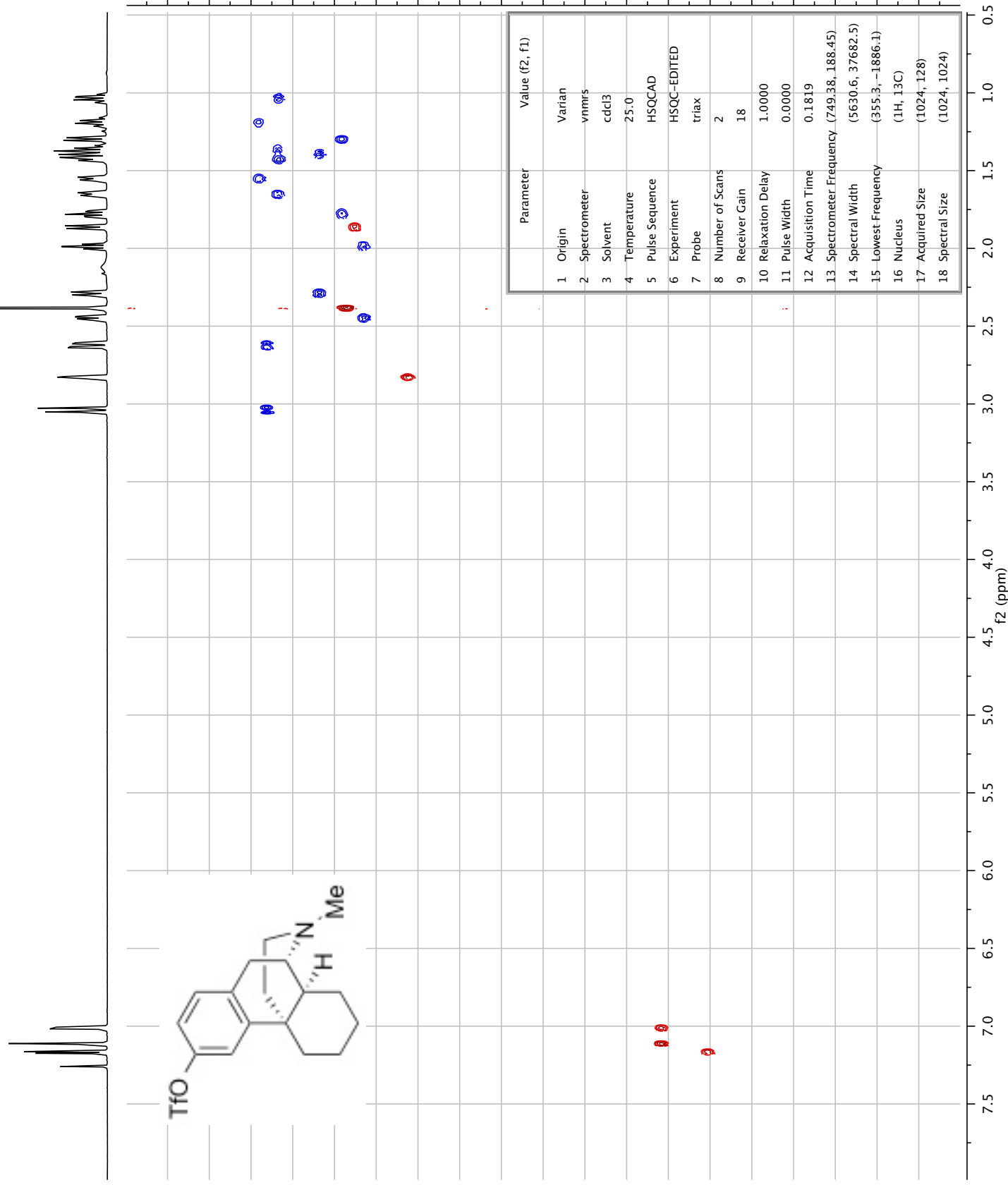
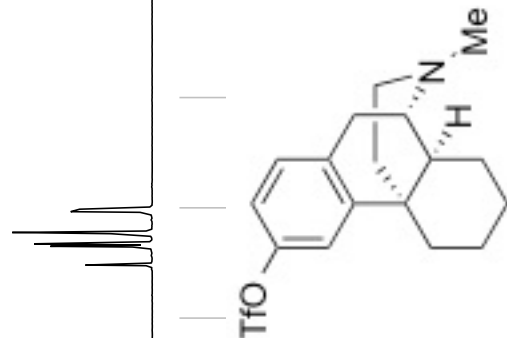
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	1326
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency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



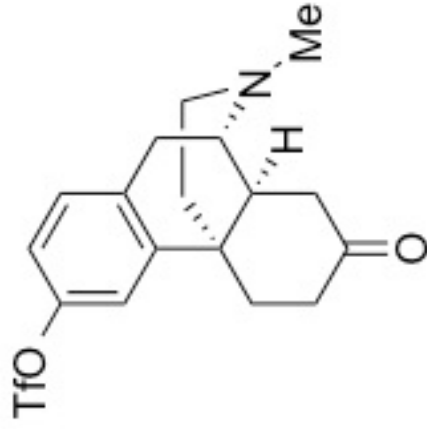




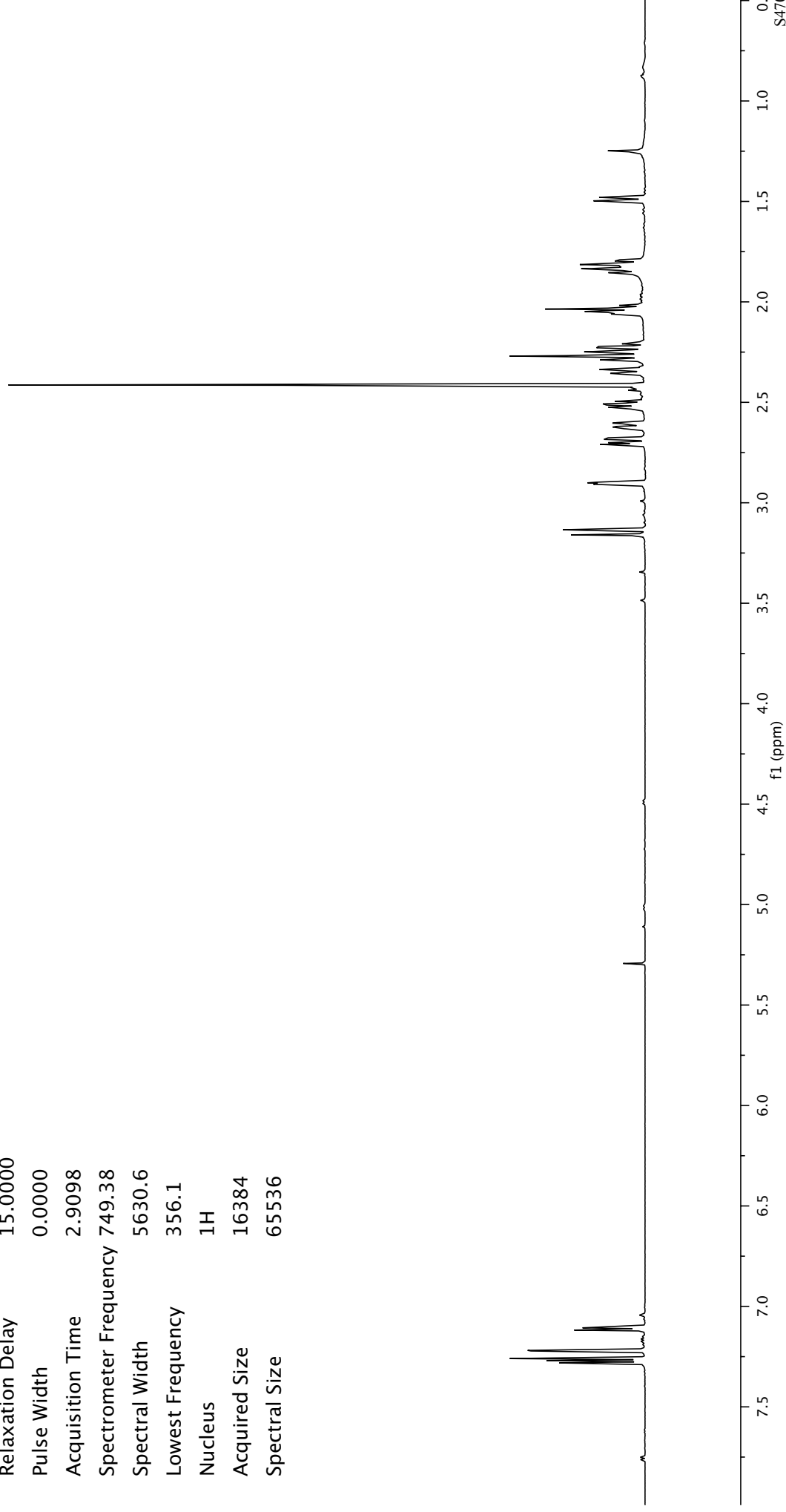
Parameter	Value (f2, f1)
1 Origin	Varian
2 Spectrometer	nmr5
3 Solvent	cdcl3
4 Temperature	25.0
5 Pulse Sequence	gCOSY
6 Experiment	COSY
7 Probe	tripax
8 Number of Scans	2
9 Receiver Gain	18
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	0.1501
13 Spectrometer Frequency	(749.38, 749.38)
14 Spectral Width	(5630.6, 5630.6)
15 Lowest Frequency	(355.3, 355.3)
16 Nucleus	(1H, 1H)
17 Acquired Size	(845, 128)
18 Spectral Size	(1024, 1024)

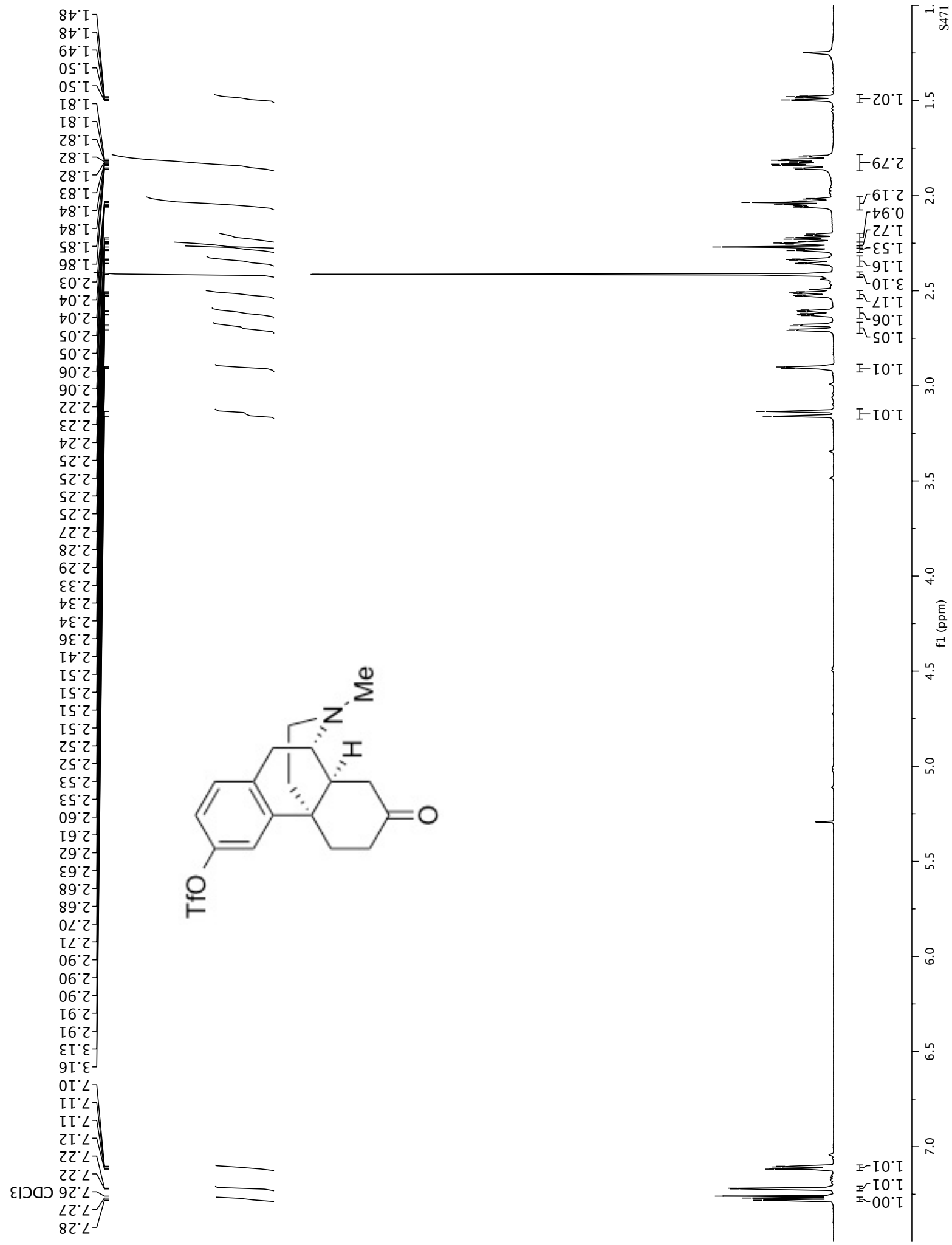


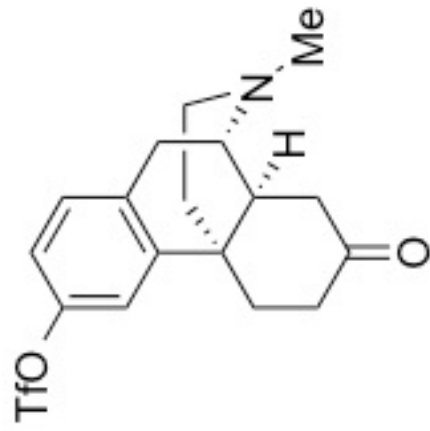
Parameter	Value (f2, f1)
1 Origin	Varian
2 Spectrometer	nmr5
3 Solvent	cdcl3
4 Temperature	25.0
5 Pulse Sequence	HSQCAD
6 Experiment	HSQC-EDITED
7 Probe	triax
8 Number of Scans	2
9 Receiver Gain	18
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	0.1819
13 Spectrometer Frequency	(749.38, 188.45)
14 Spectral Width	(5630.6, 37682.5)
15 Lowest Frequency	(355.3, -1886.1)
16 Nucleus	(^1H , ^{13}C)
17 Acquired Size	(1024, 128)
18 Spectral Size	(1024, 1024)



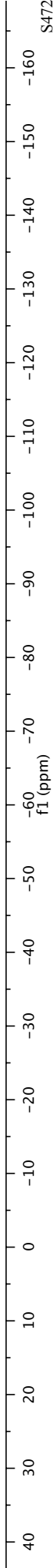
Parameter	Value
Origin	Varian
Spectrometer	vmnrs
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	triax
Number of Scans	16
Receiver Gain	32
Relaxation Delay	15.0000
Pulse Width	0.0000
Acquisition Time	2.9098
Spectrometer Frequency	749.38
Spectral Width	5630.6
Lowest Frequency	356.1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

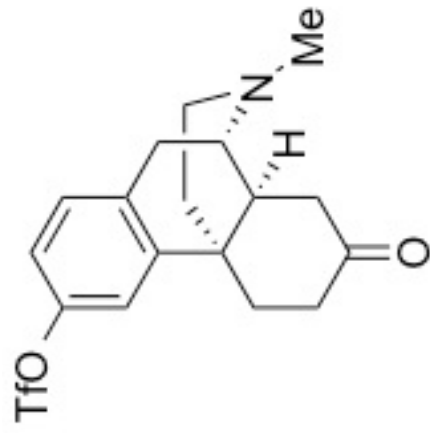




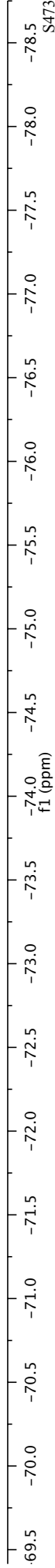


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	128
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency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





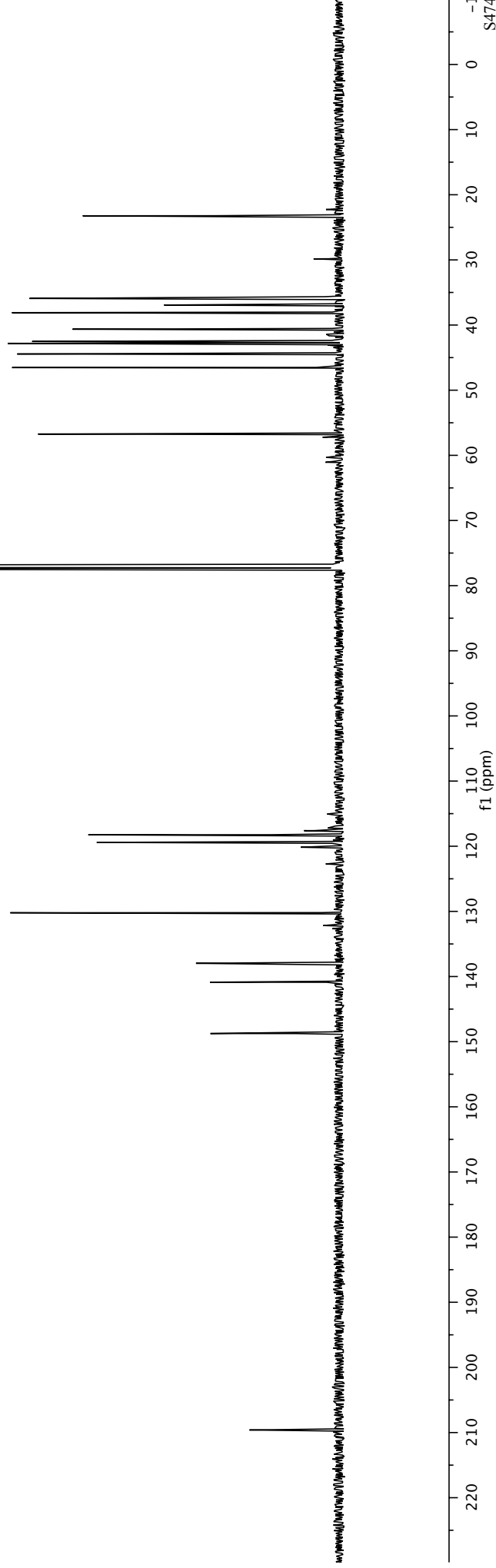
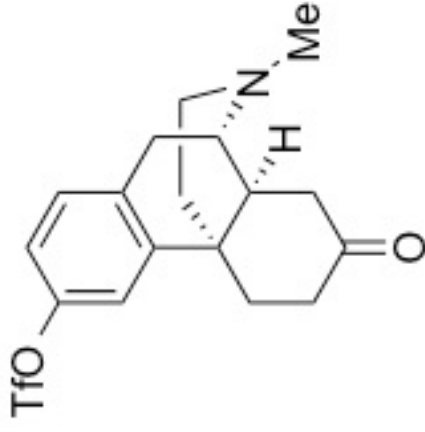
--73.14

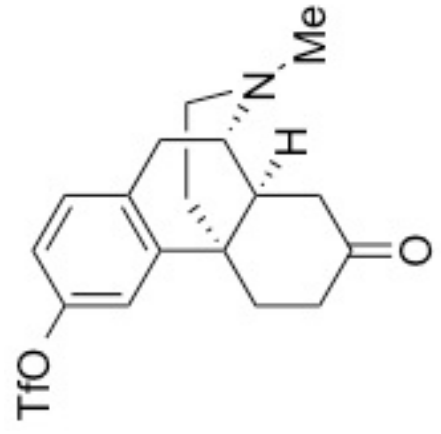
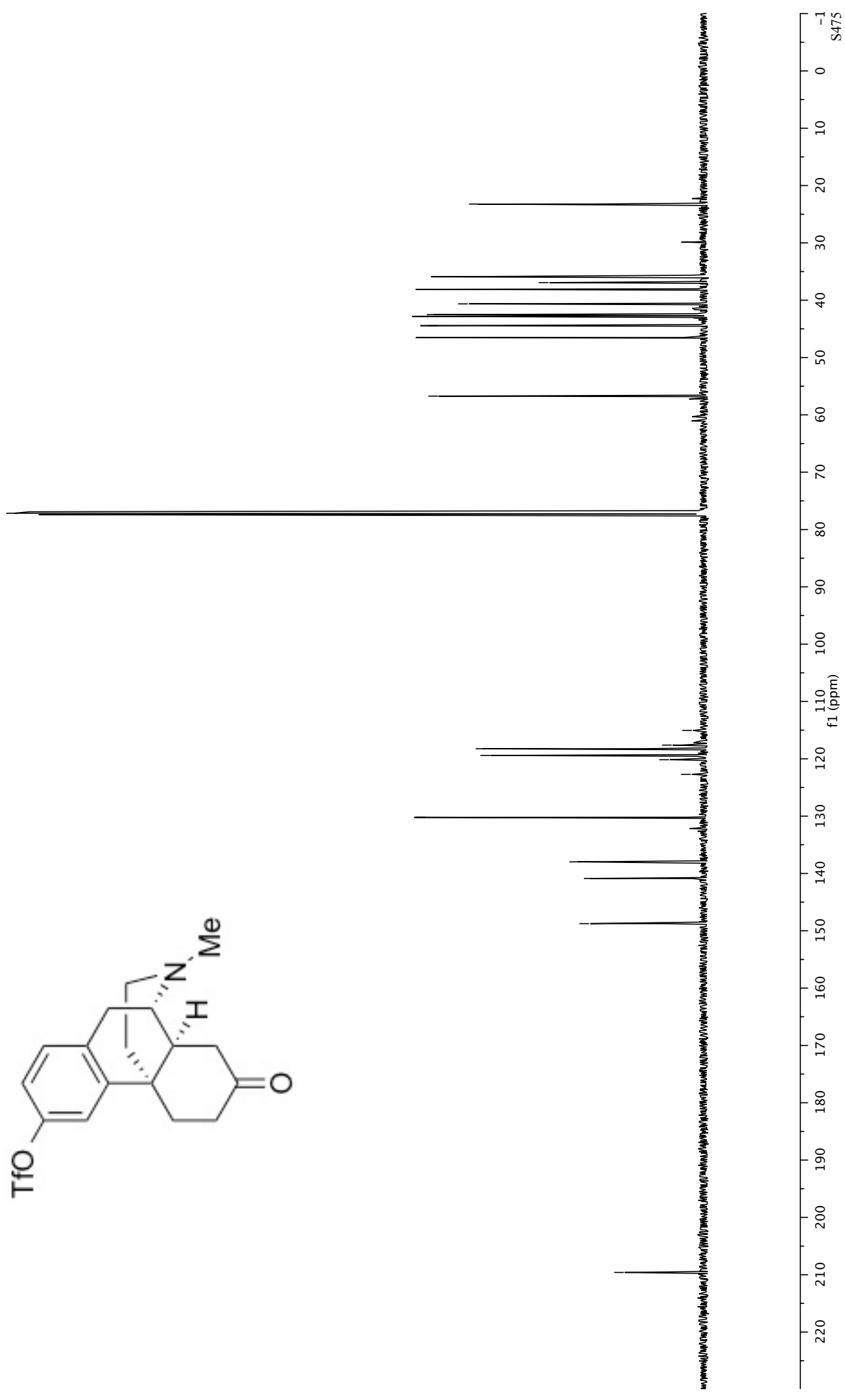


Parameter

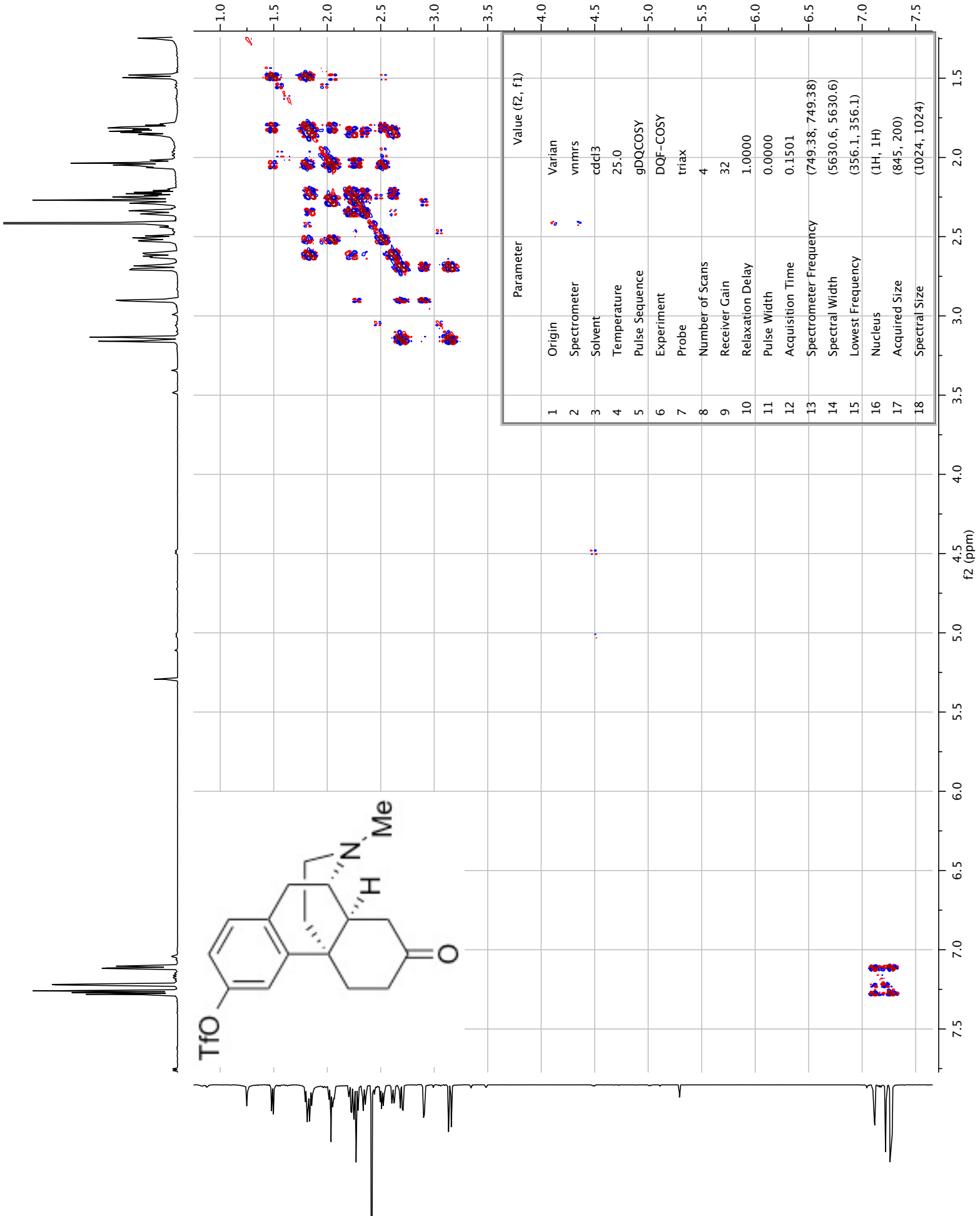
Value

Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
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	¹³ C
Acquired Size	32768
Spectral Size	65536

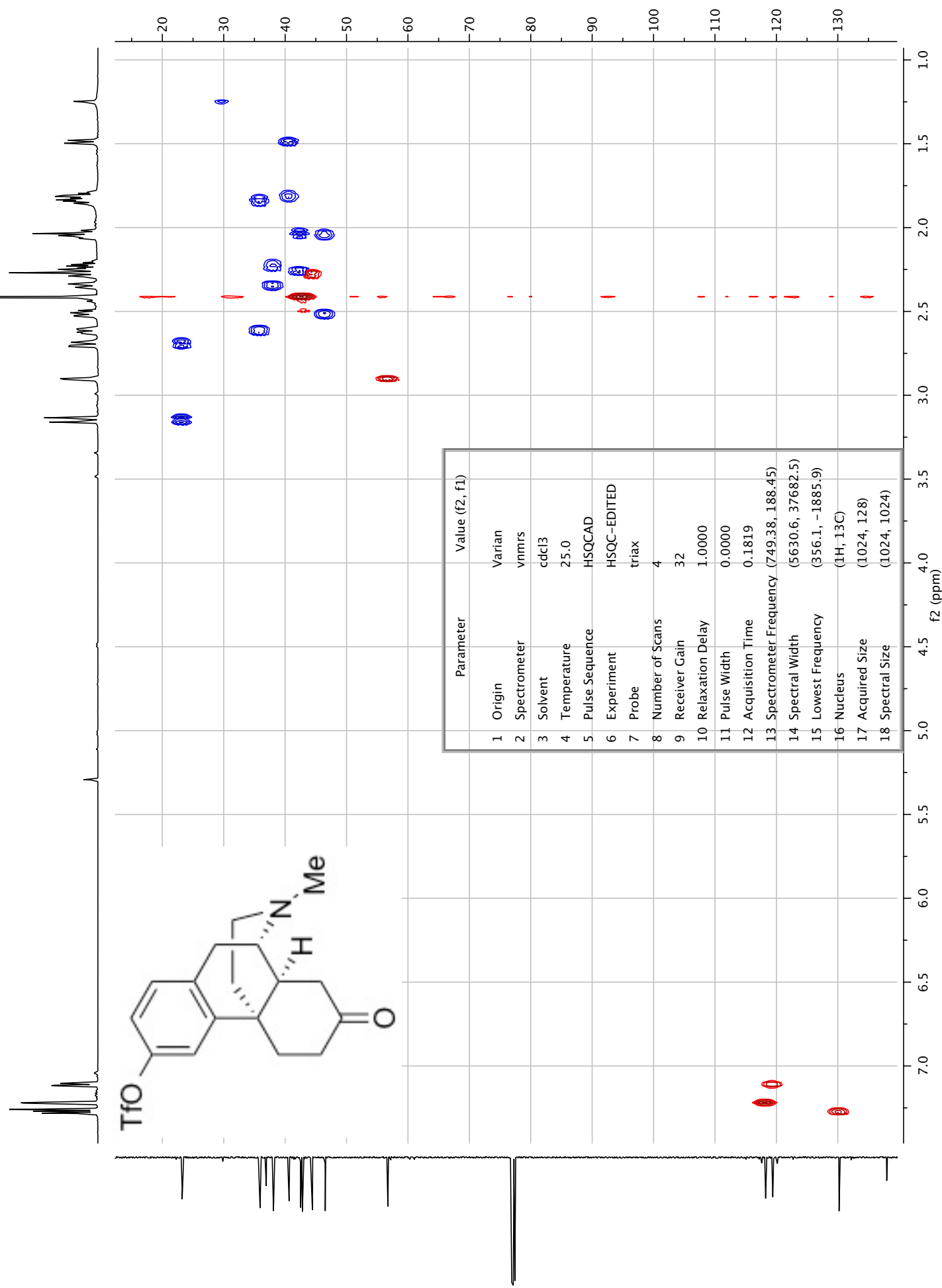


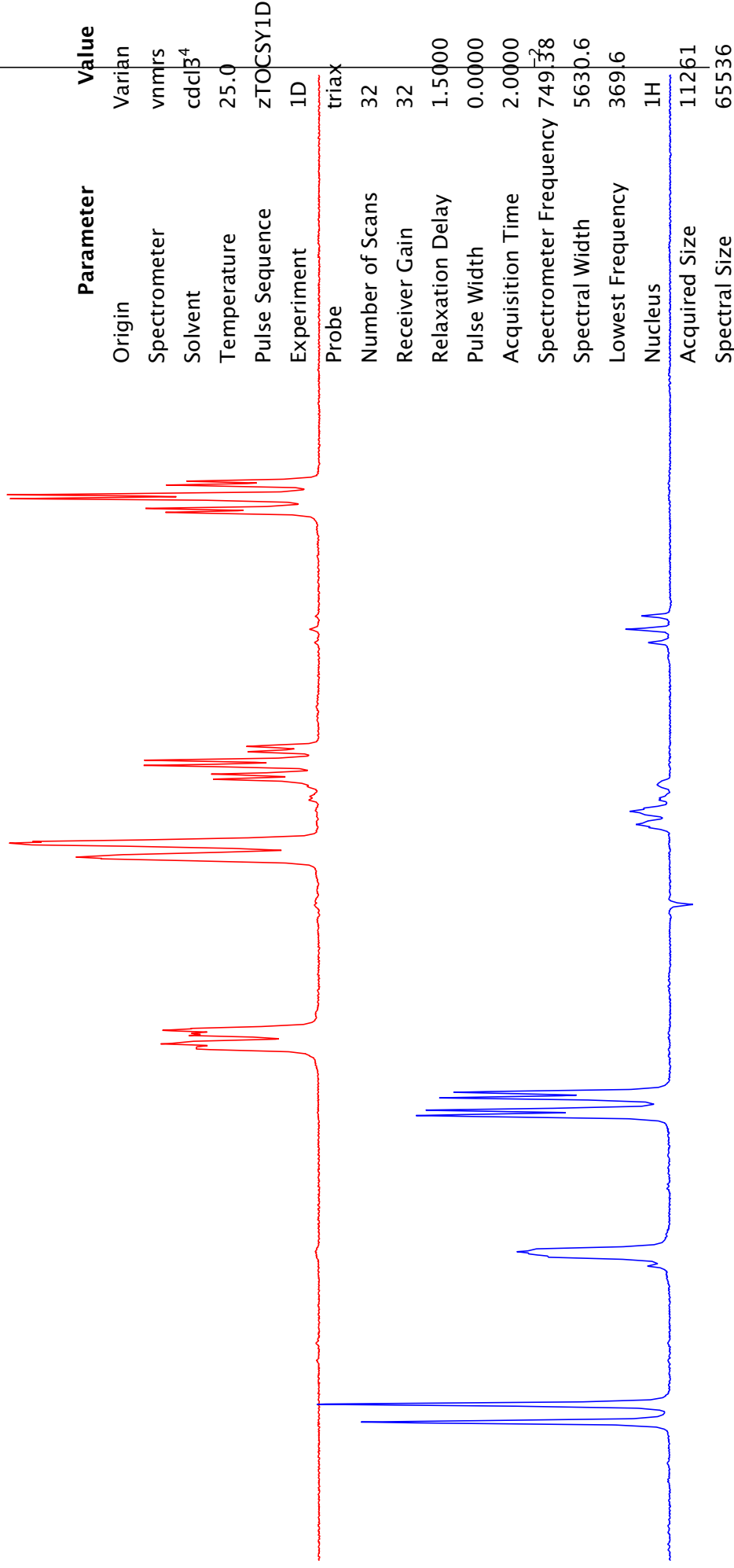
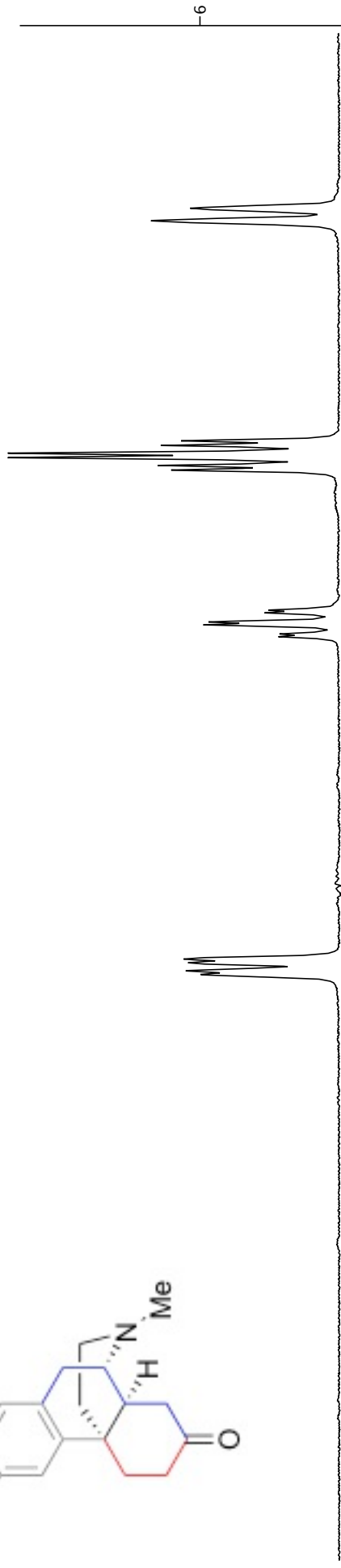
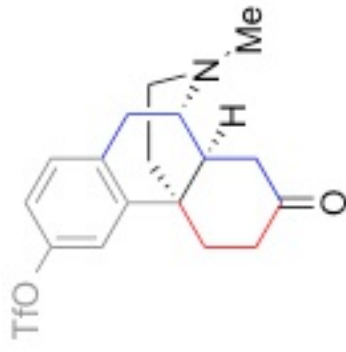


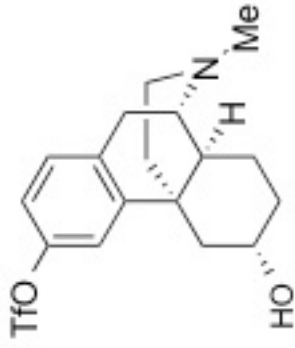
- 209.61
- 148.75
- 140.87
- 137.98
- 130.22
- 122.71
- 120.16
- 119.42
- 118.25
- 117.61
- 115.05
- 77.16 CDCl₃
- 56.73
- 46.53
- 44.44
- 42.81
- 42.52
- 40.64
- 38.10
- 36.93
- 35.92
- 23.23



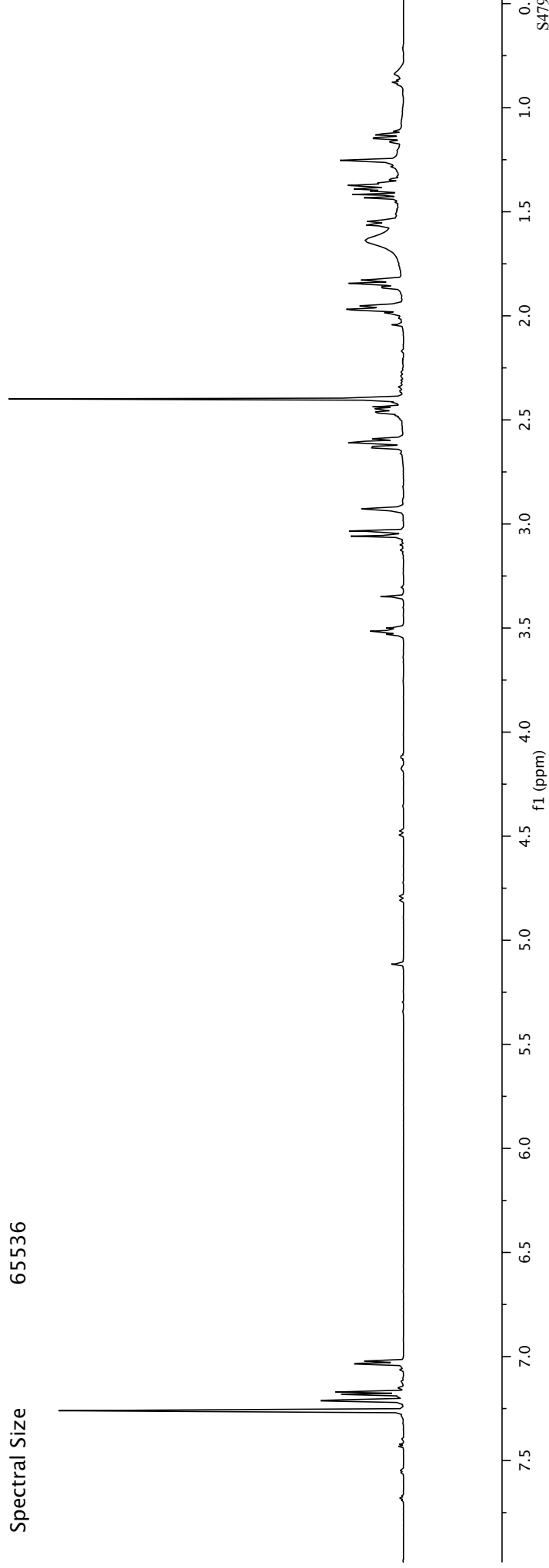
	Parameter	Value (f2, f1)
1	Origin	
2	Spectrometer	Varian
3	Solvent	vnmr5
4	Temperature	cdcl3
5	Pulse Sequence	25.0
6	Experiment	gDQCOSY
7	Probe	DQF-COSY
8	Number of Scans	triax
9	Receiver Gain	4
10	Relaxation Delay	32
11	Pulse Width	1.0000
12	Acquisition Time	0.0000
13	Spectrometer Frequency	0.1501
14	Spectral Width	(749.38, 749.38)
15	Lowest Frequency	(5630.6, 5630.6)
16	Nucleus	(356.1, 356.1)
17	Acquired Size	(1H, 1H)
18	Spectral Size	(845, 200)
		(1024, 1024)



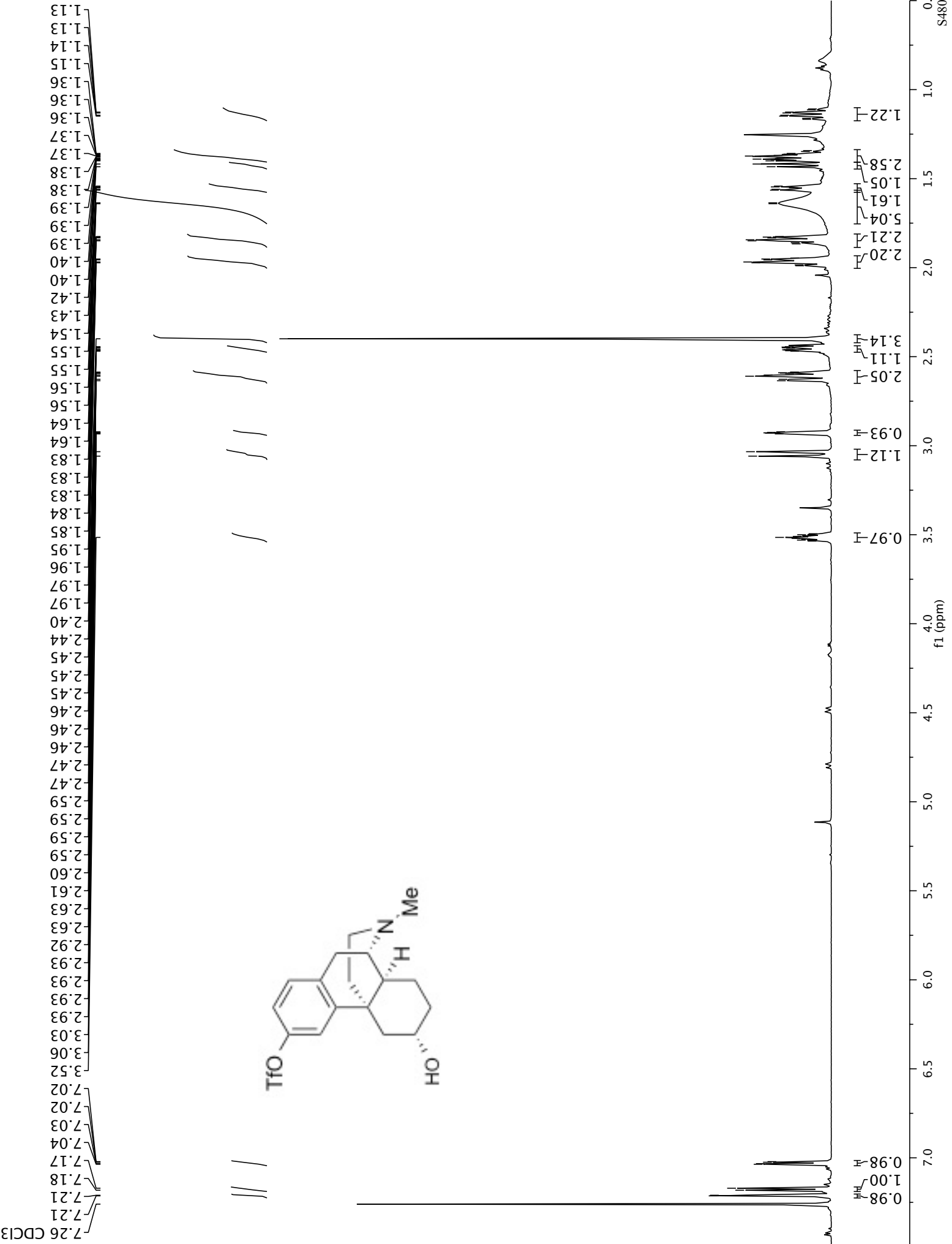


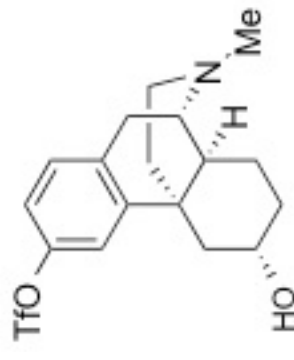


Parameter	Value
Origin	Varian
Spectrometer	vmrs
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	triax
Number of Scans	16
Receiver Gain	32
Relaxation Delay	15.0000
Pulse Width	0.0000
Acquisition Time	2.9098
Spectrometer Frequency	749.38
Spectral Width	5630.6
Lowest Frequency	356.1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

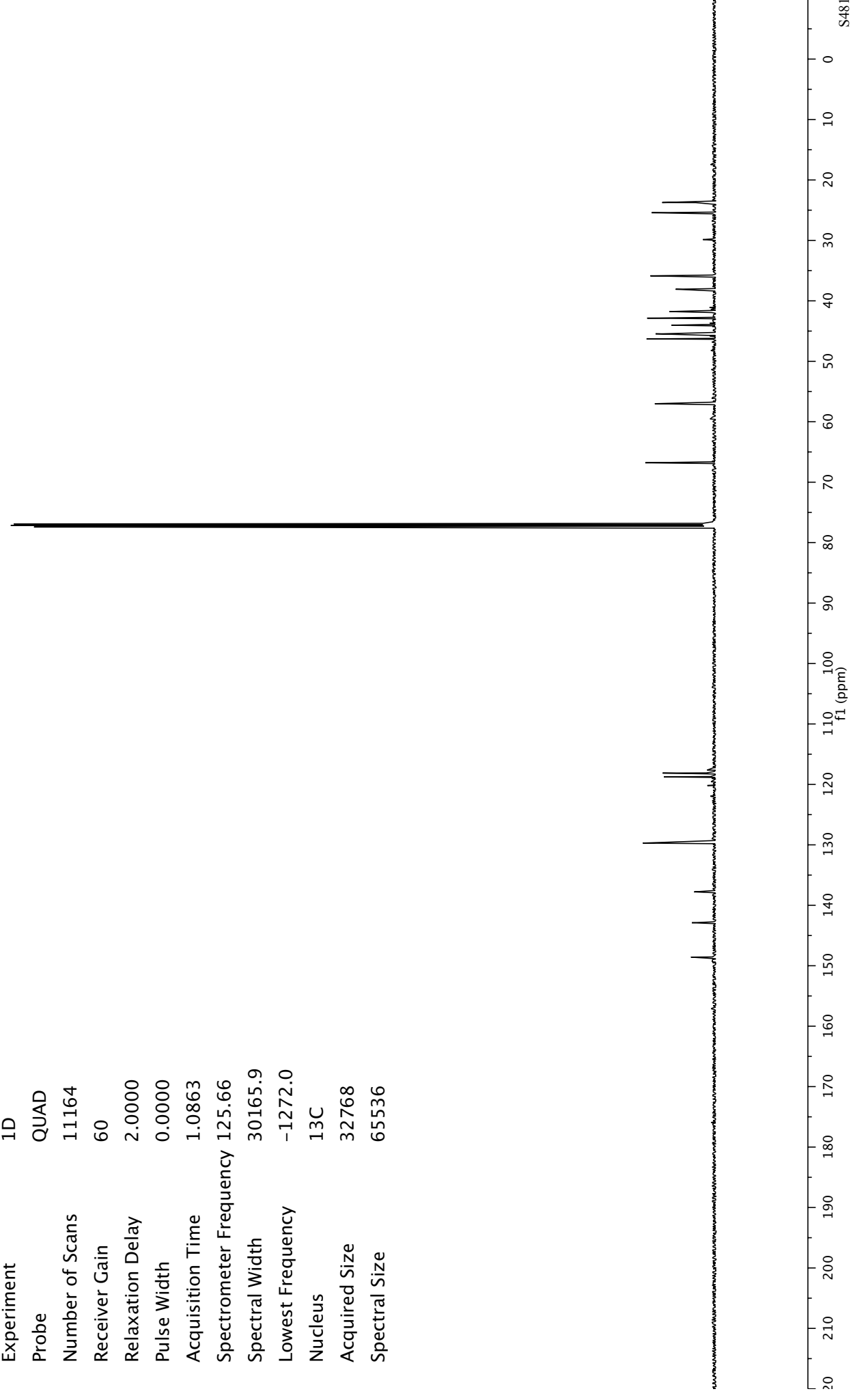


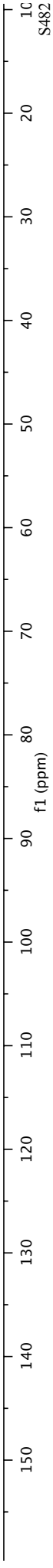
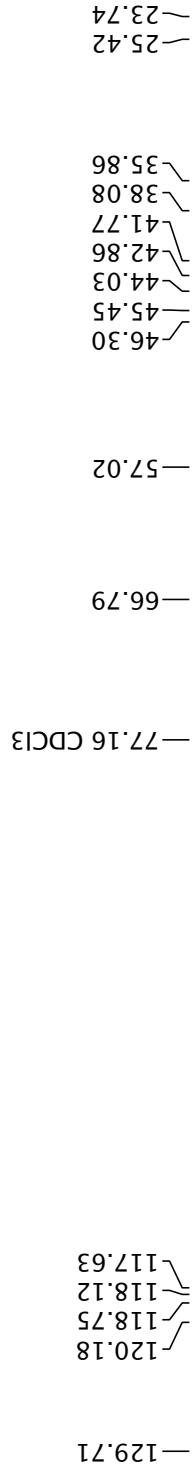
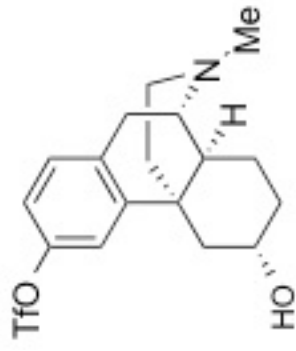
7.26 CDCl₃

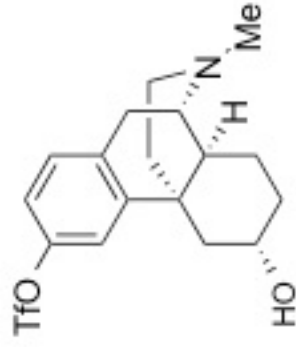




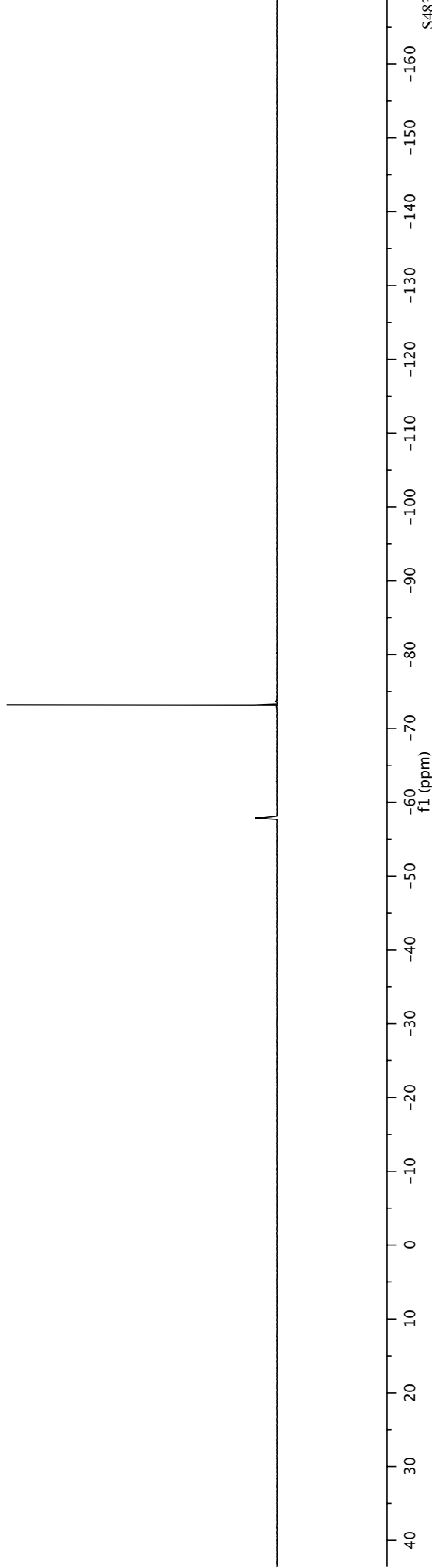
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	11164
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1272.0
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

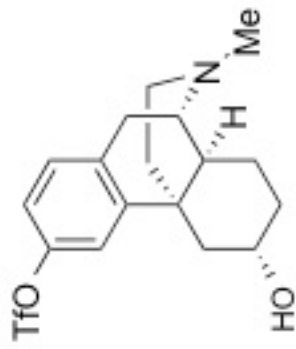




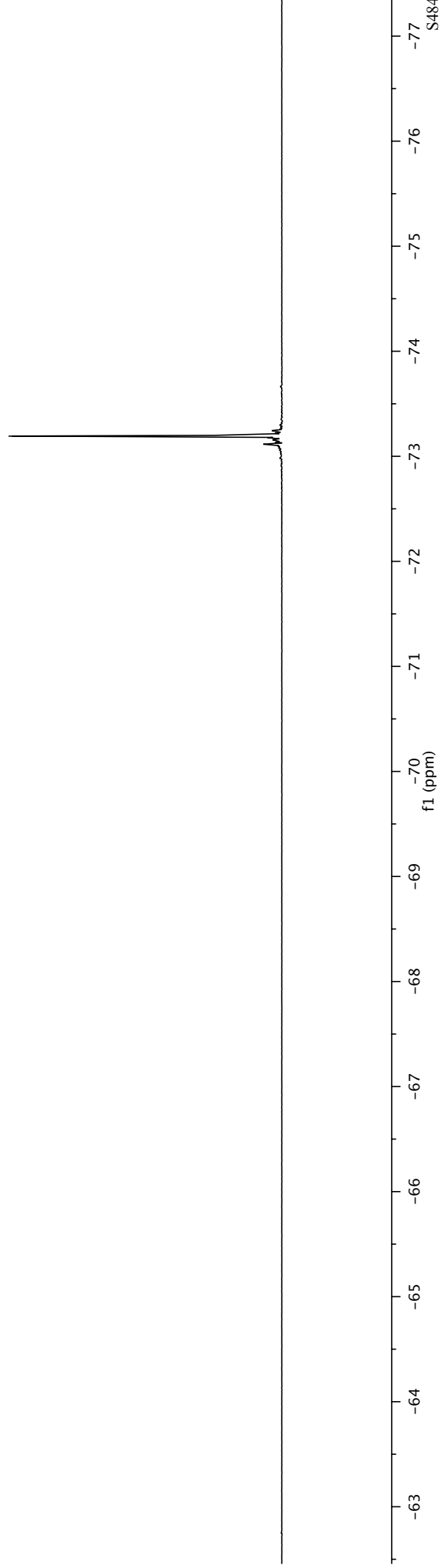


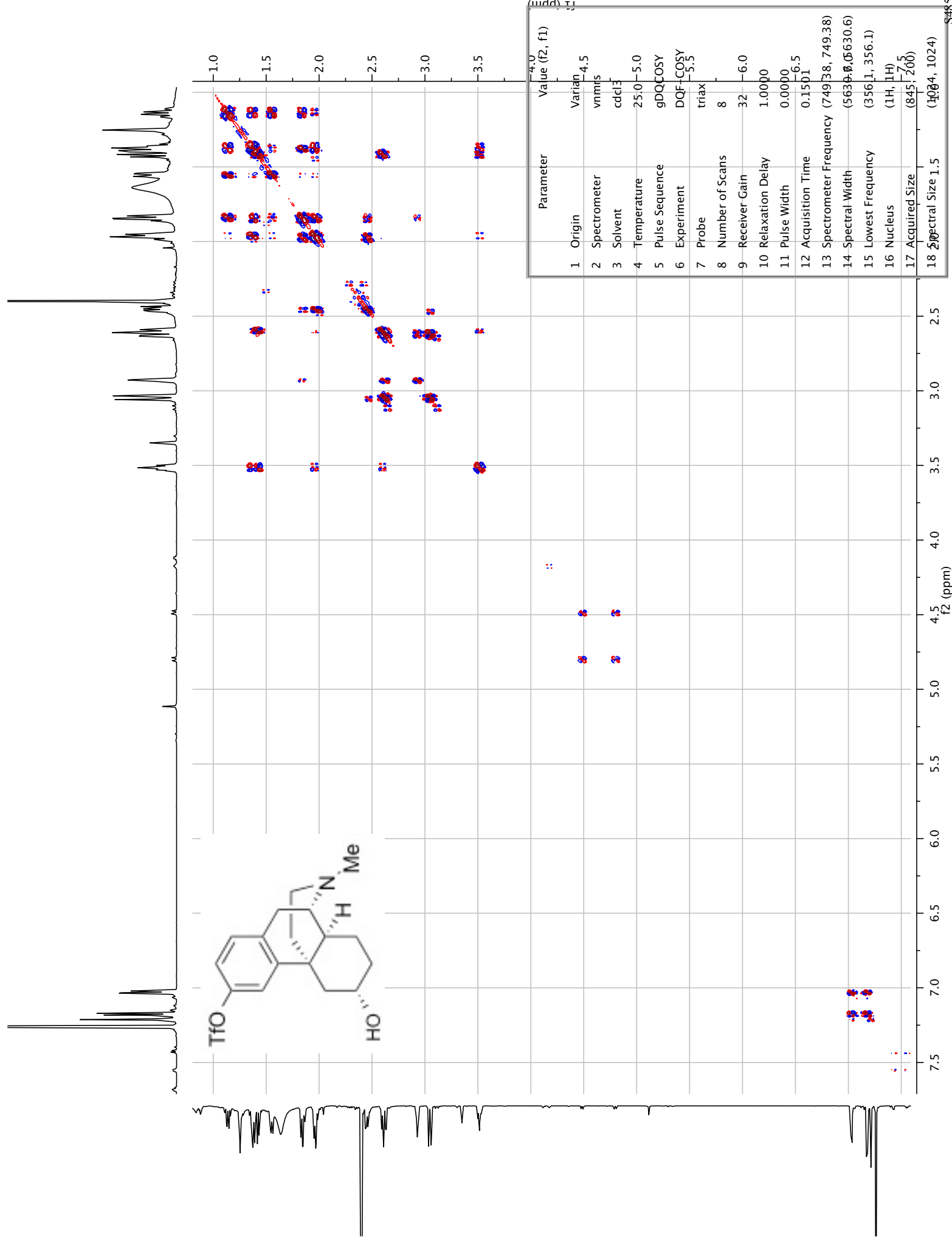
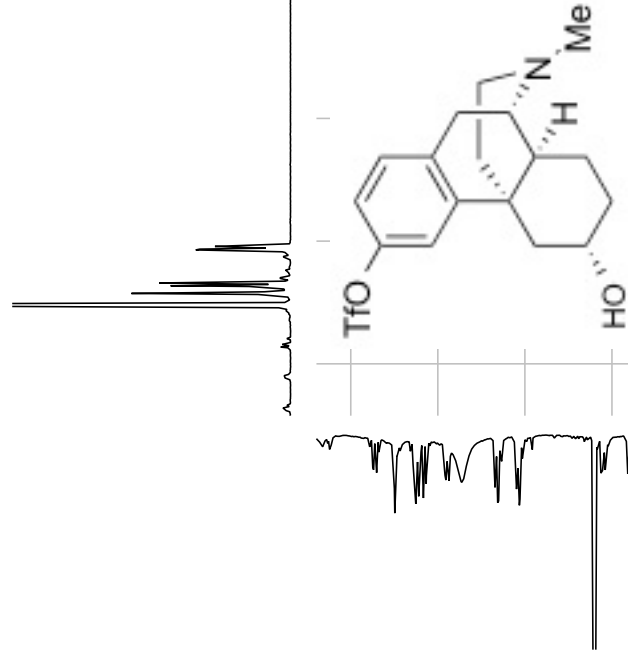
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	128
Receiver Gain	50
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	0.3277
Spectrometer Frequency	470.15
Spectral Width	100000.0
Lowest Frequency	-79501.3
Nucleus	19F
Acquired Size	32768
Spectral Size	65536



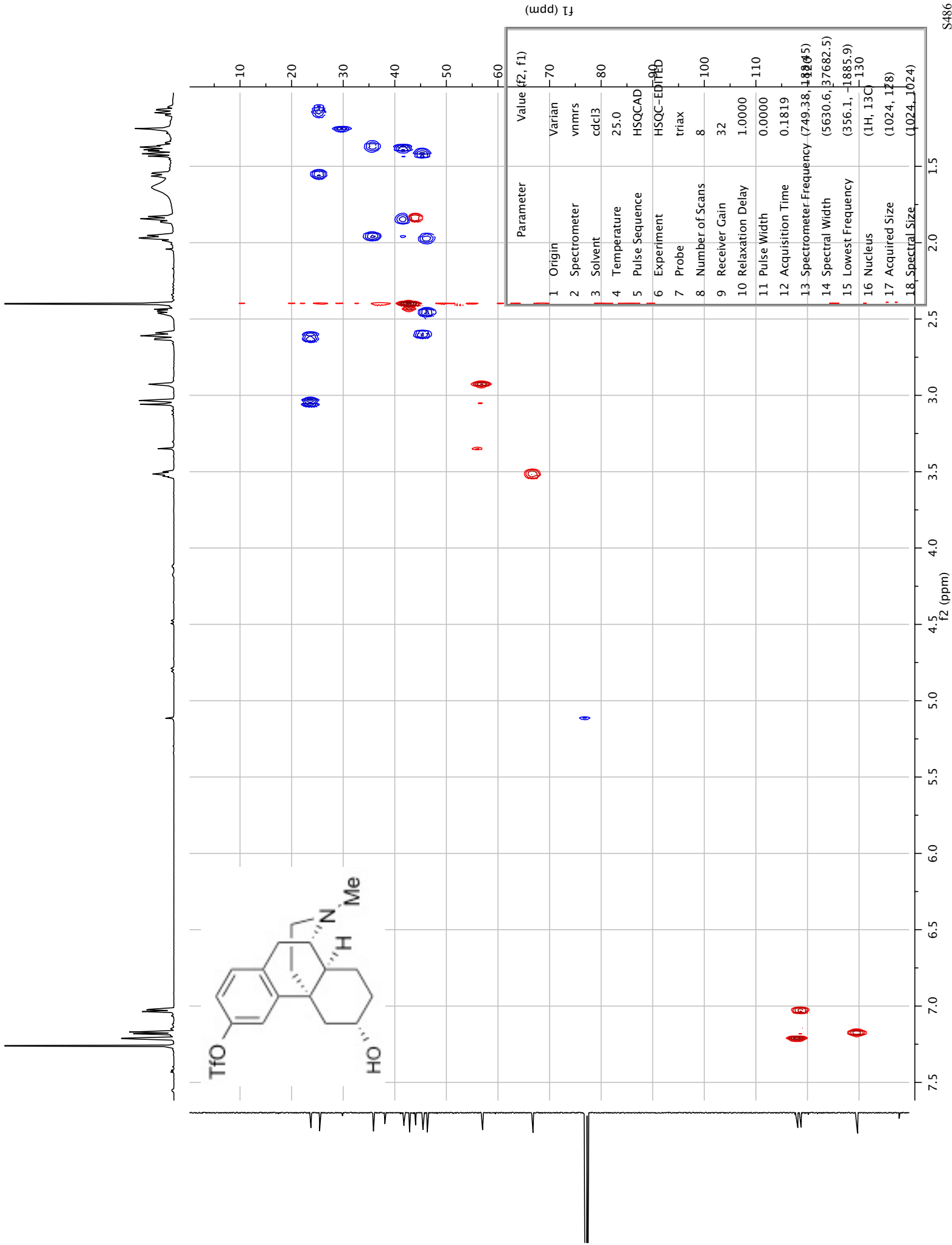


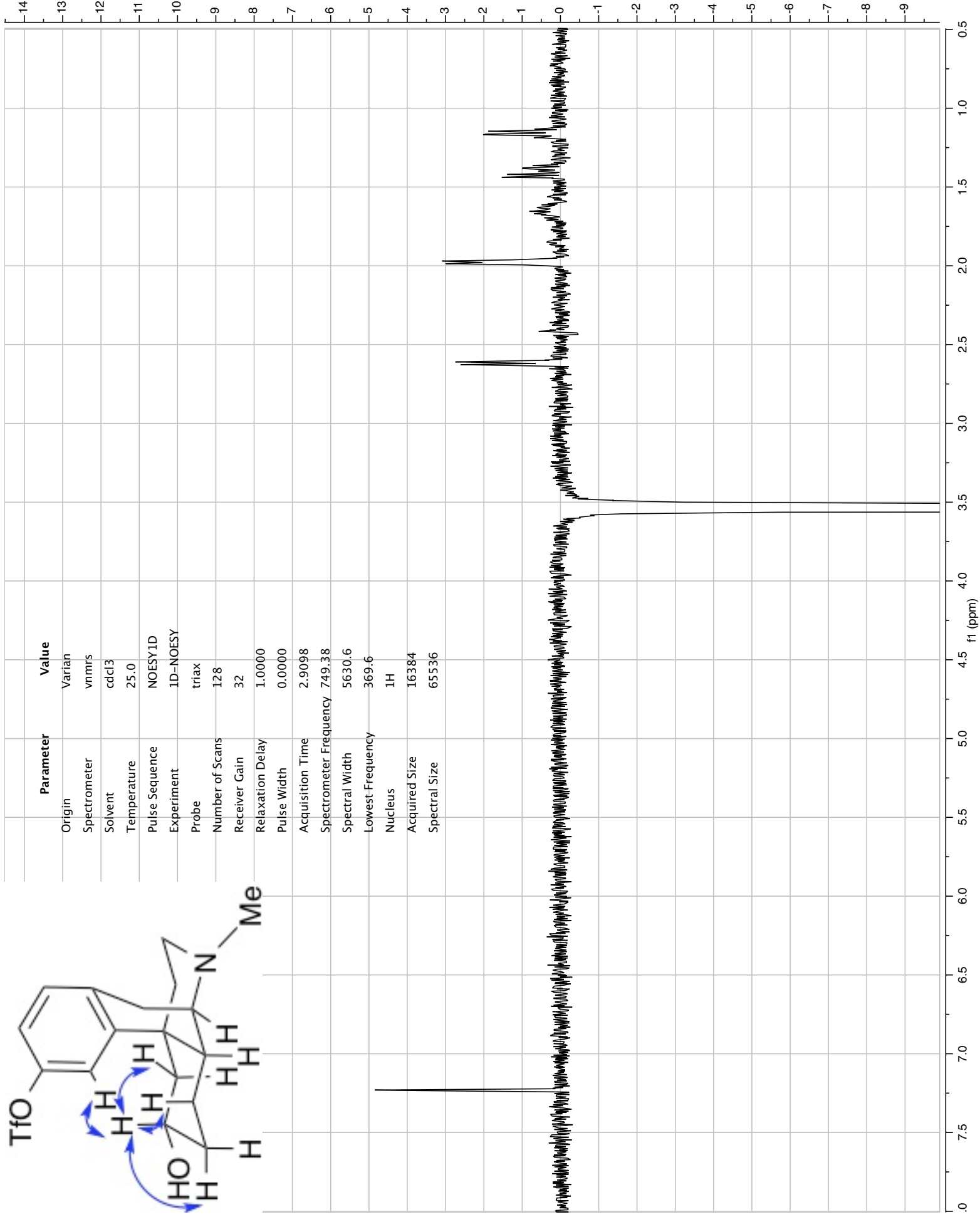
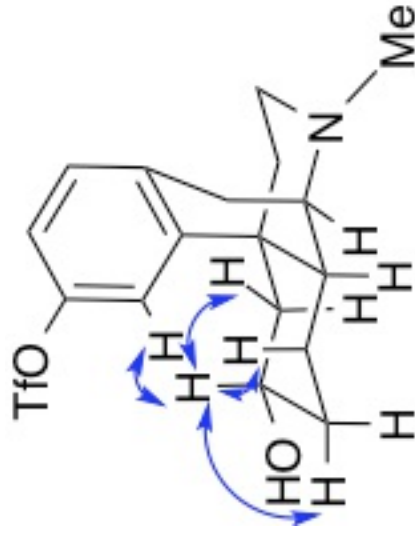
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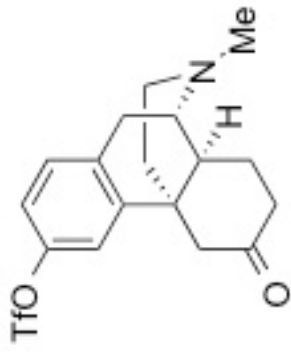




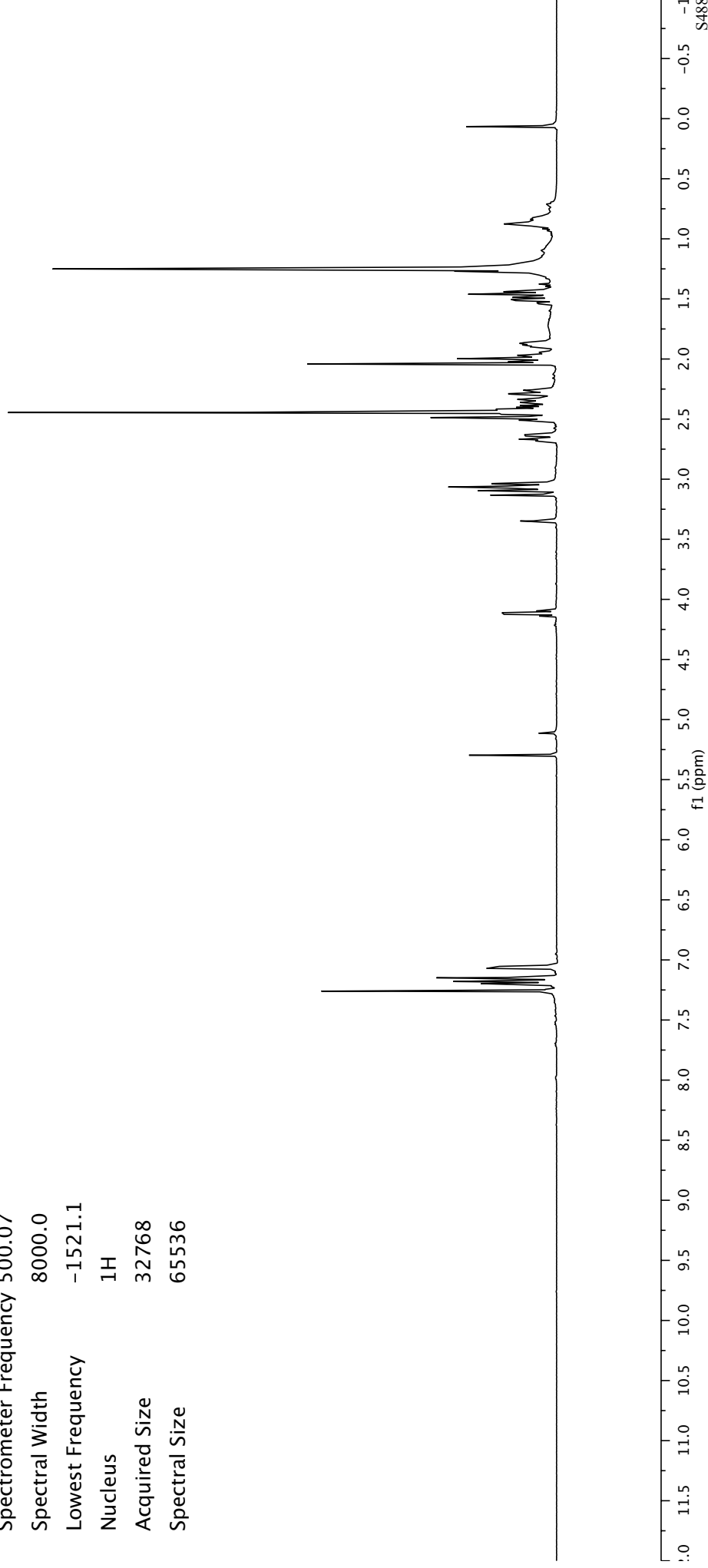
Parameter	Value (f2, f1)
1 Origin	Varian
2 Spectrometer	Varian
3 Solvent	nmr
4 Temperature	25.0
5 Pulse Sequence	gDQF-COSY
6 Experiment	DQF-COSY
7 Probe	tripax
8 Number of Scans	8
9 Receiver Gain	32
10 Relaxation Delay	1.000
11 Pulse Width	0.000
12 Acquisition Time	0.1501
13 Spectrometer Frequency (749.38, 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)	

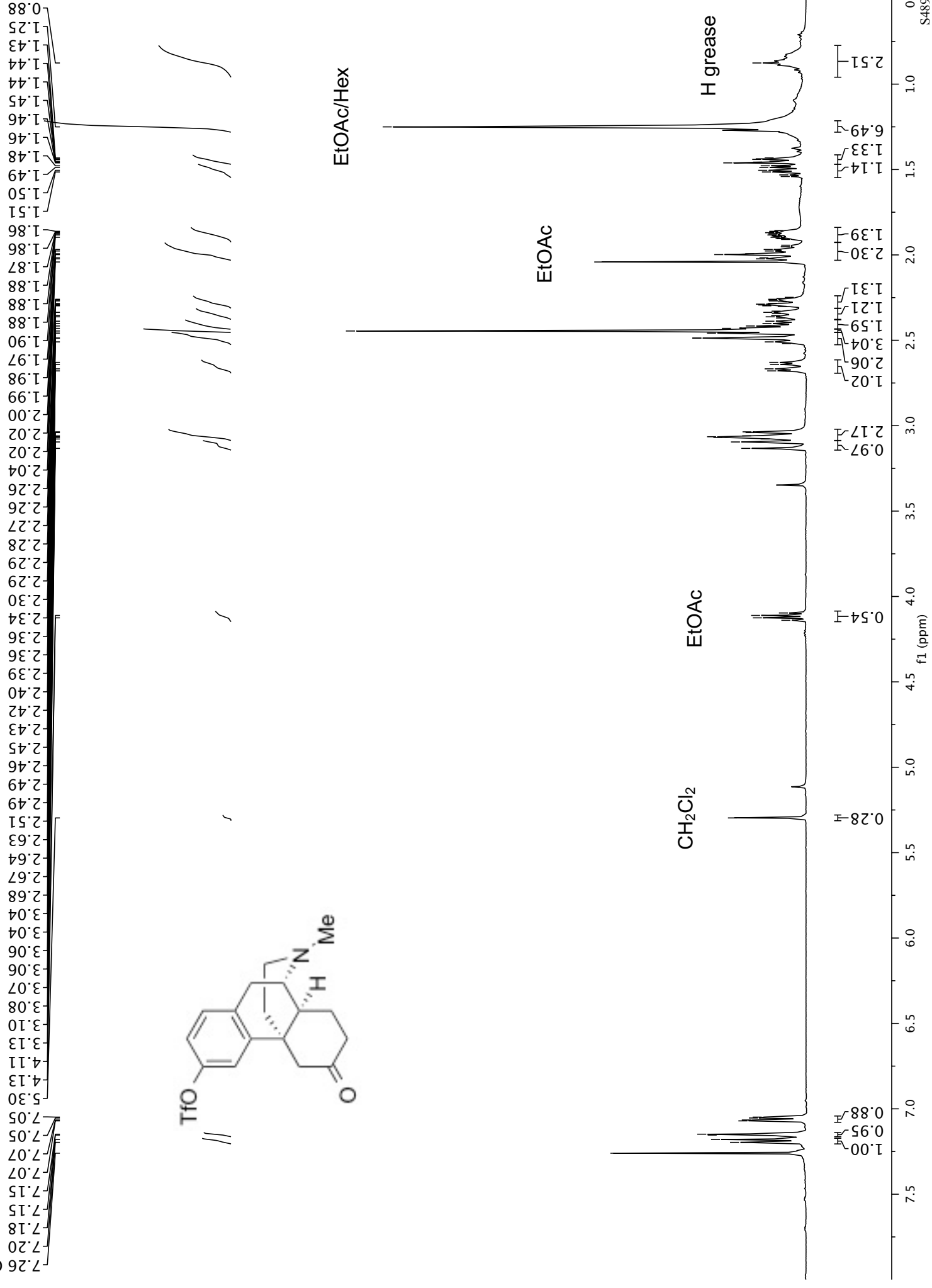
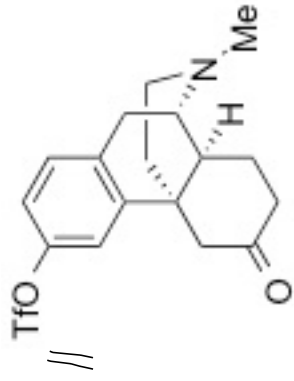


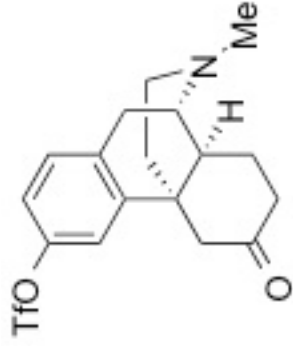




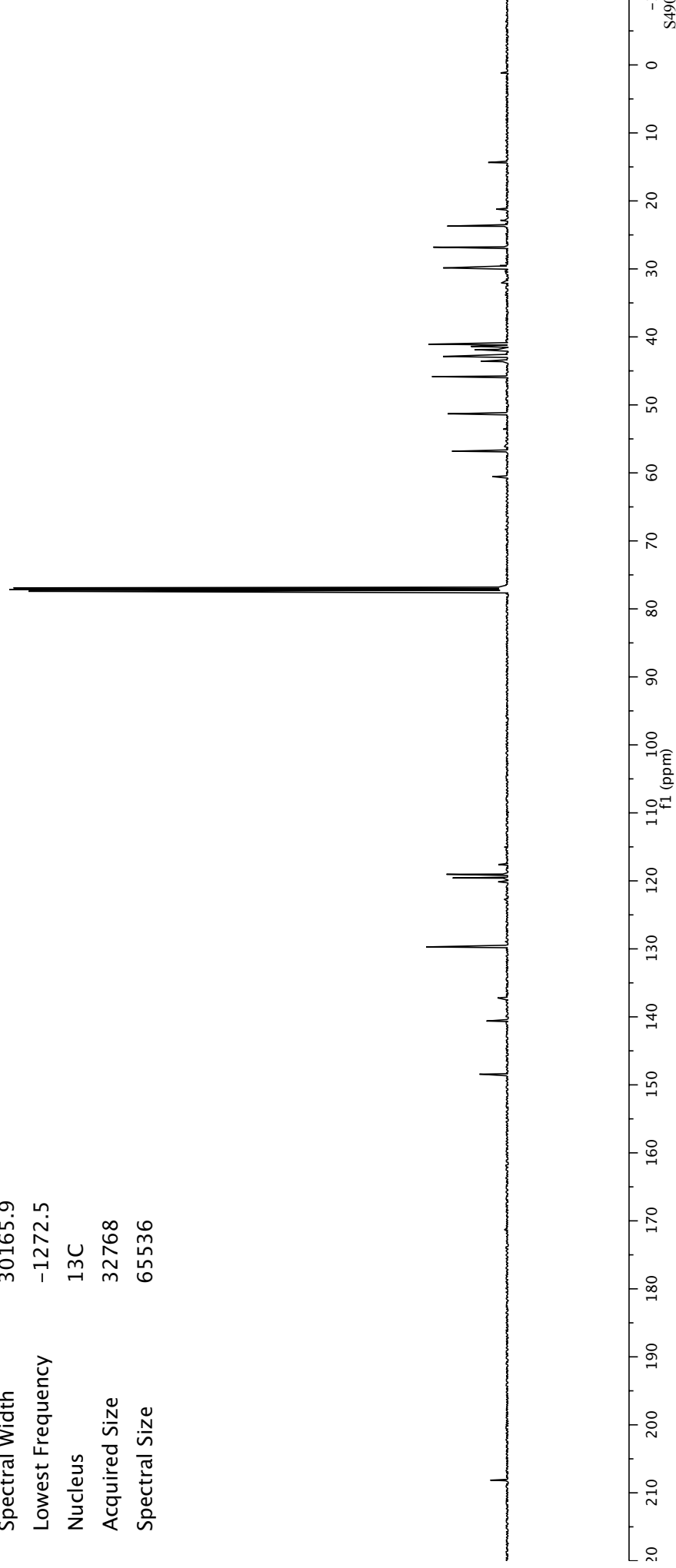
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	50.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Number of Scans	16
Receiver Gain	32
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1521.1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

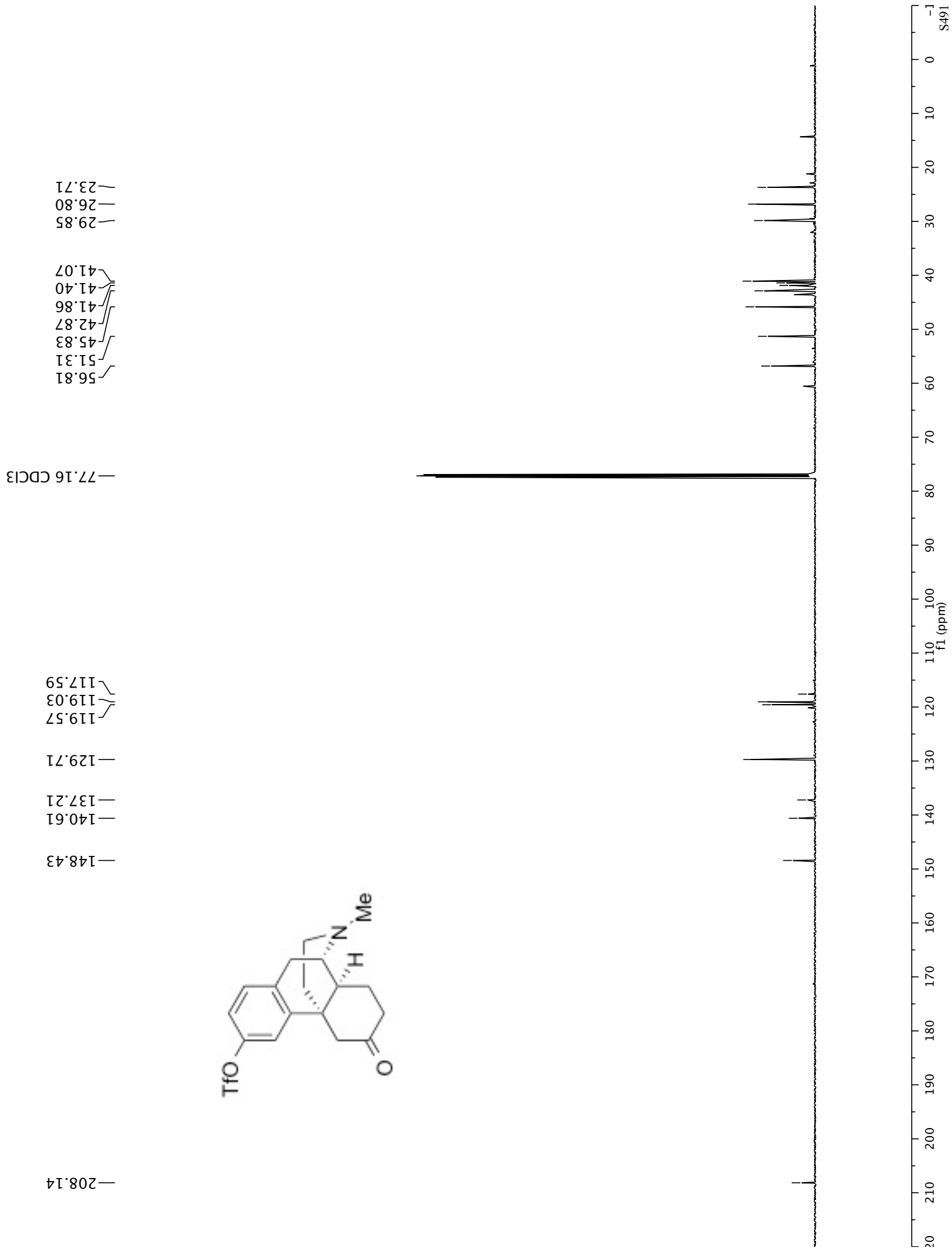


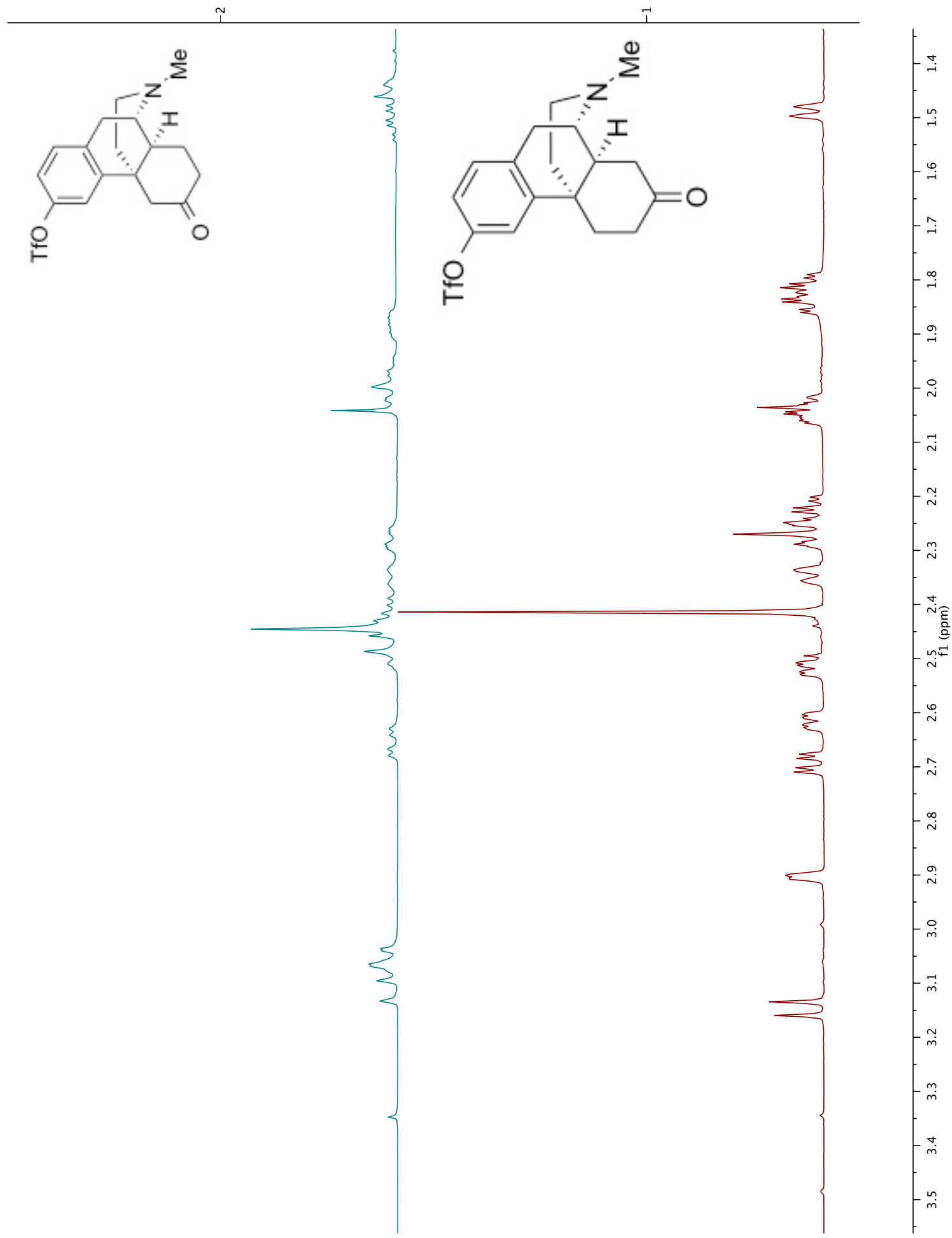




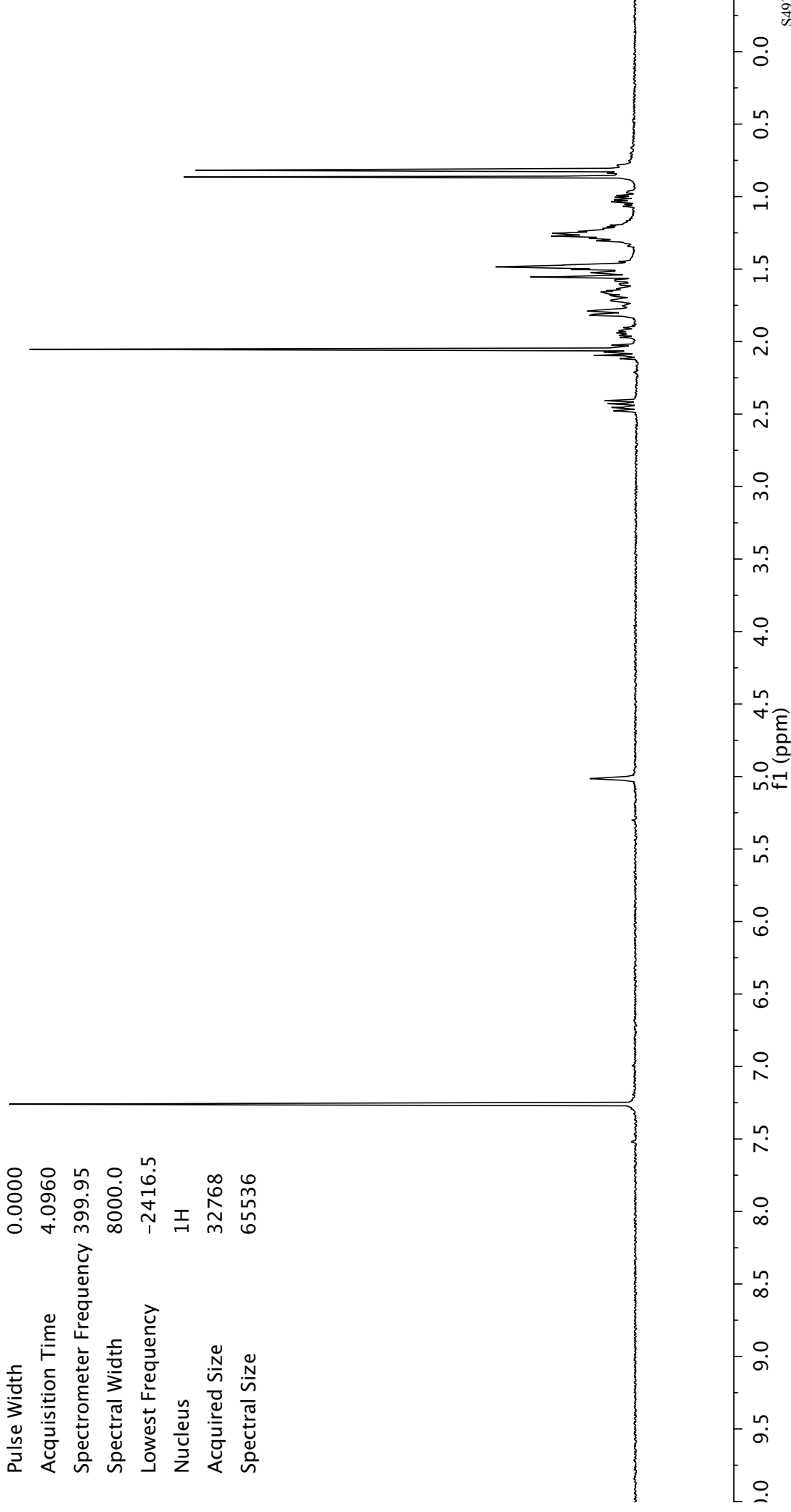
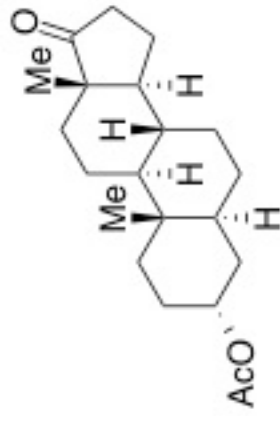
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	50.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Number of Scans	14167
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1272.5
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

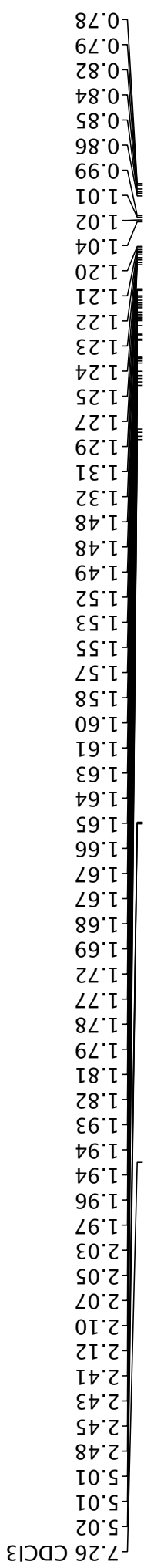
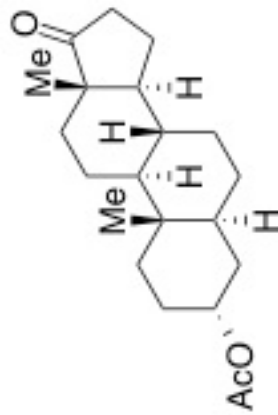
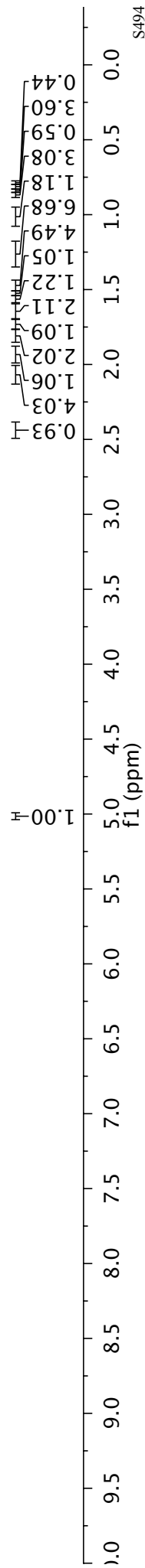


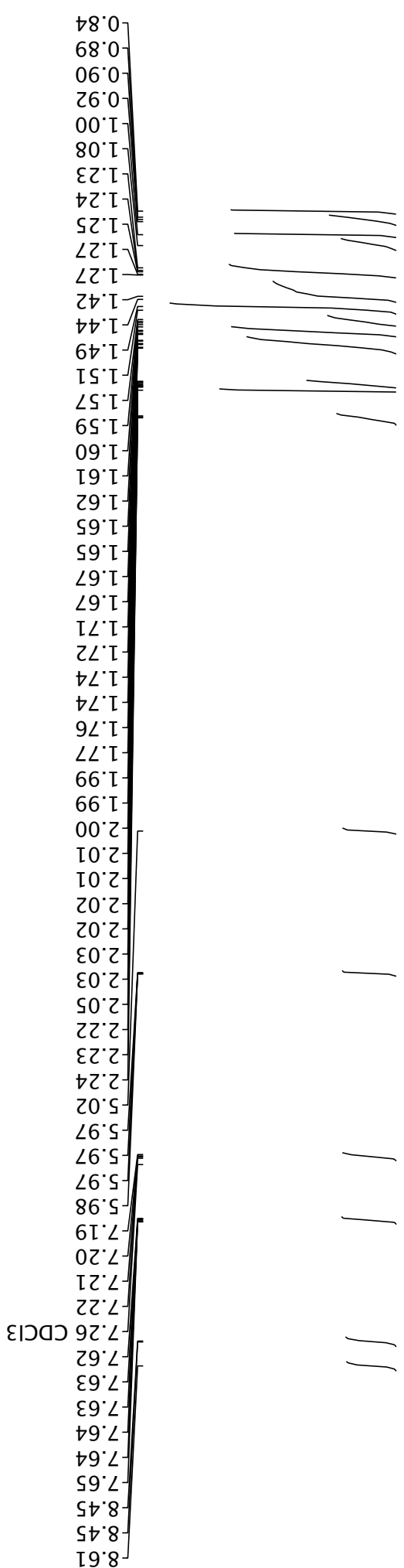
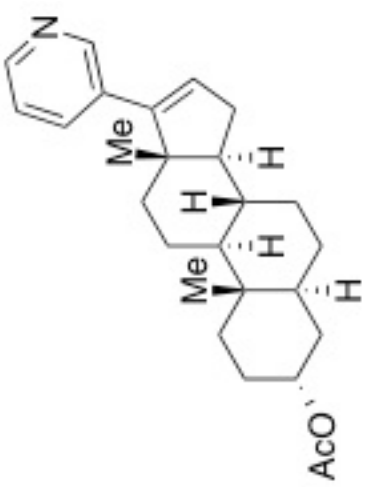
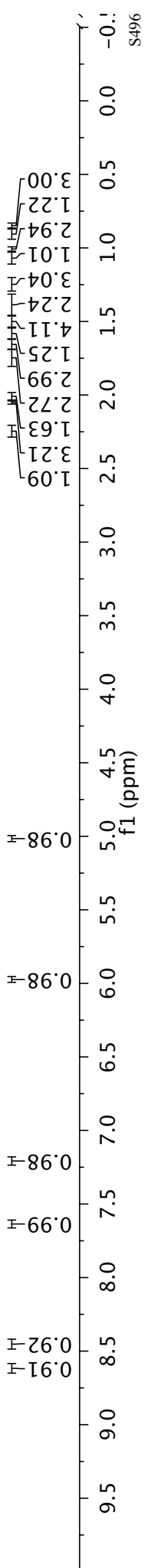


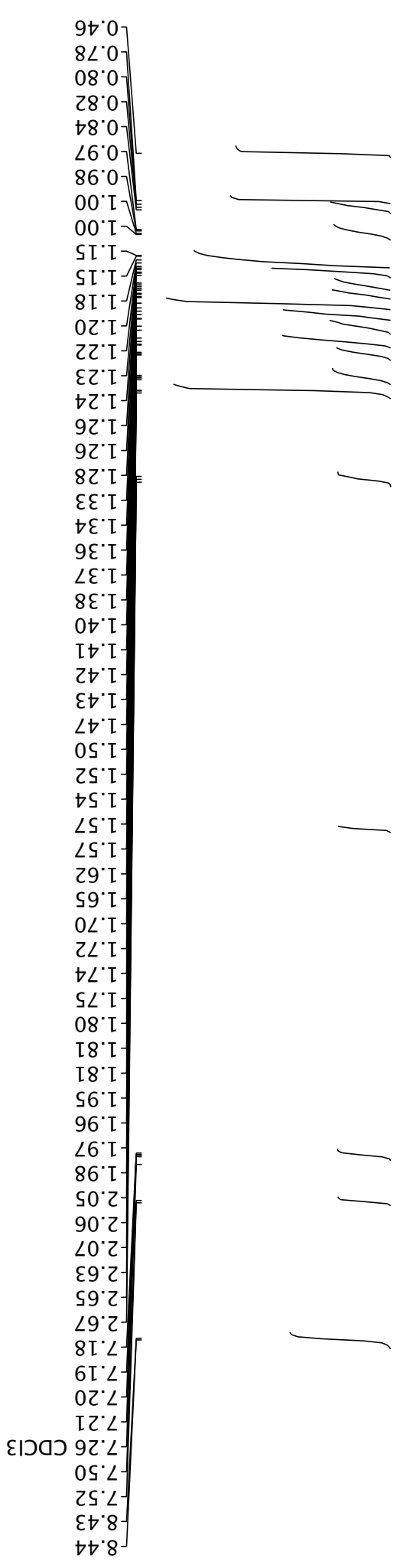
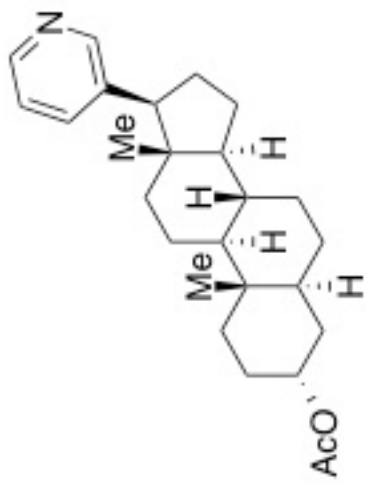
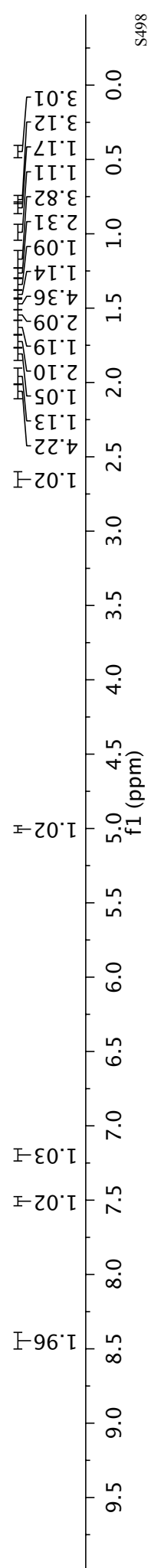


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	60
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	399.95
Spectral Width	8000.0
Lowest Frequency	-2416.5
Nucleus	¹ H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

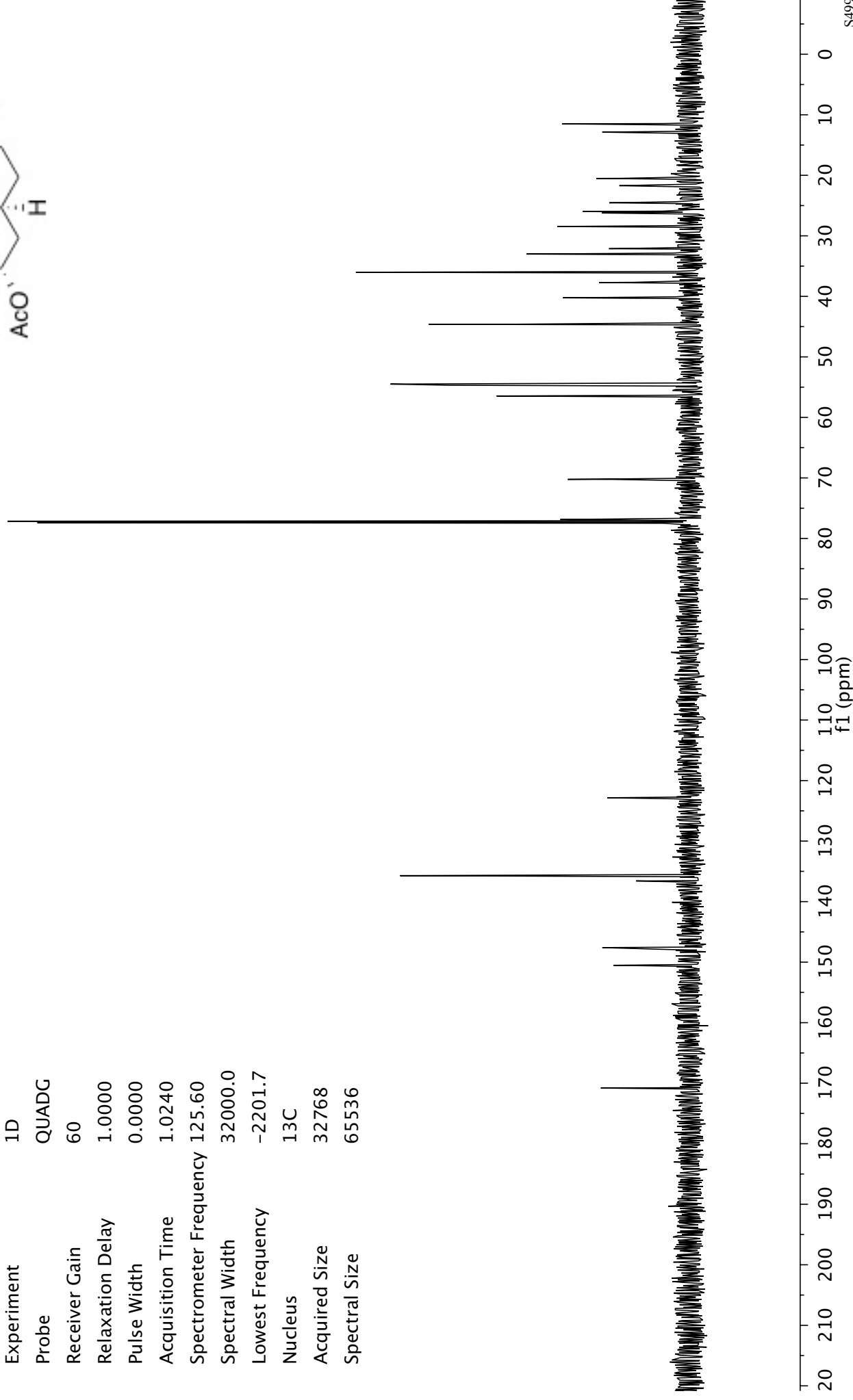
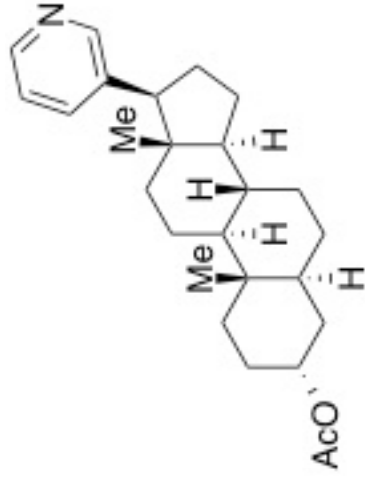


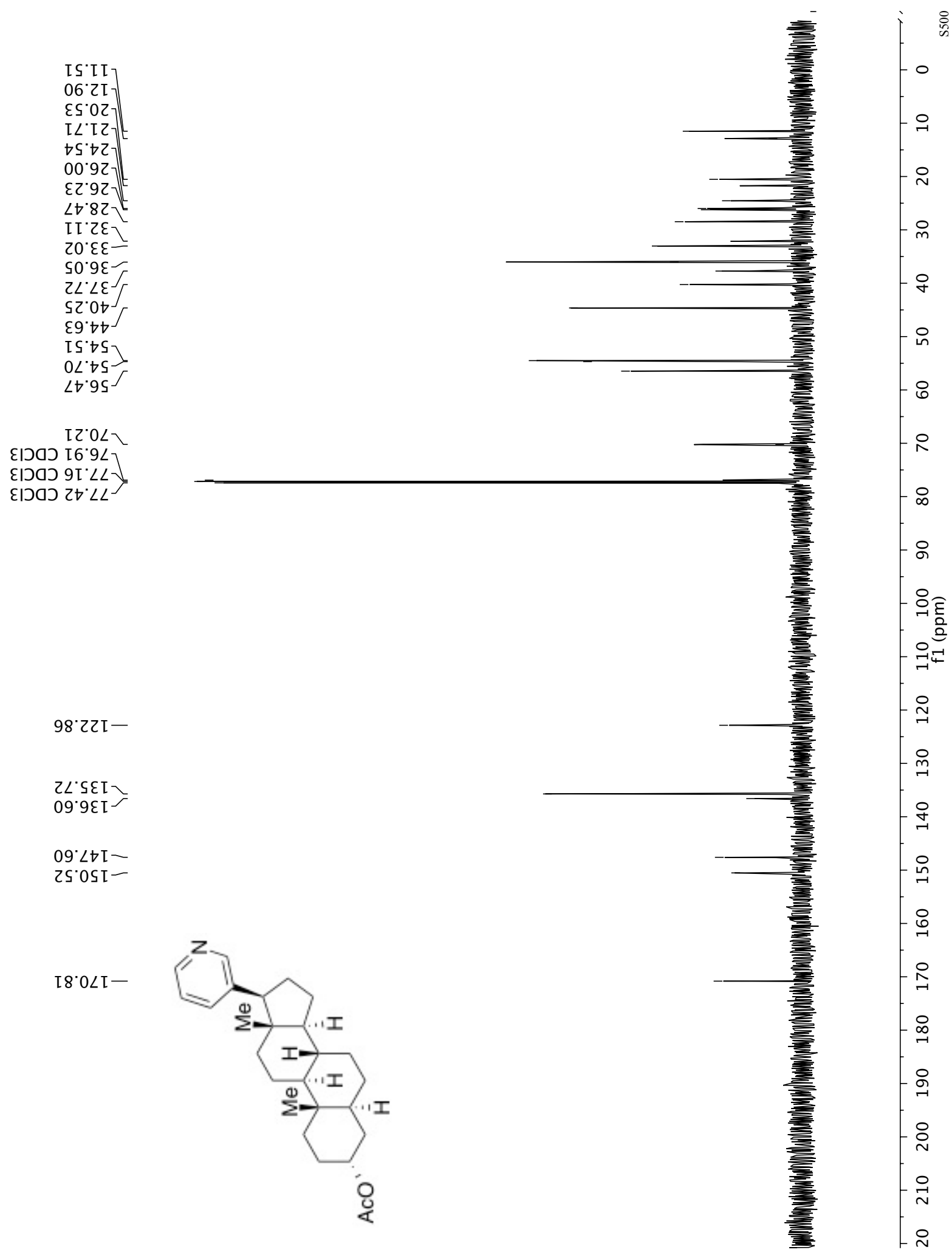


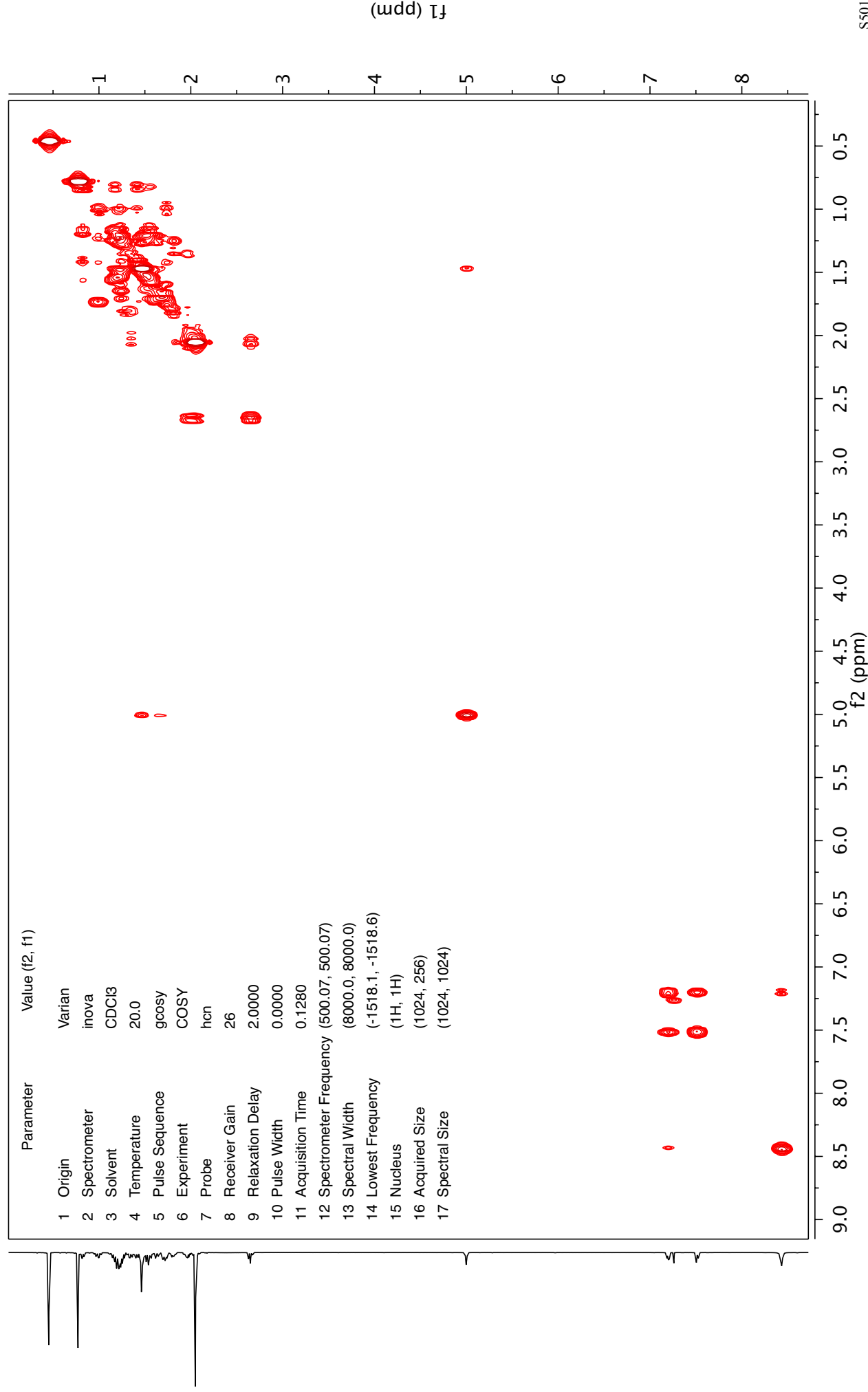
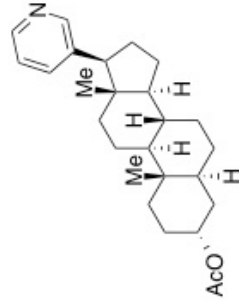


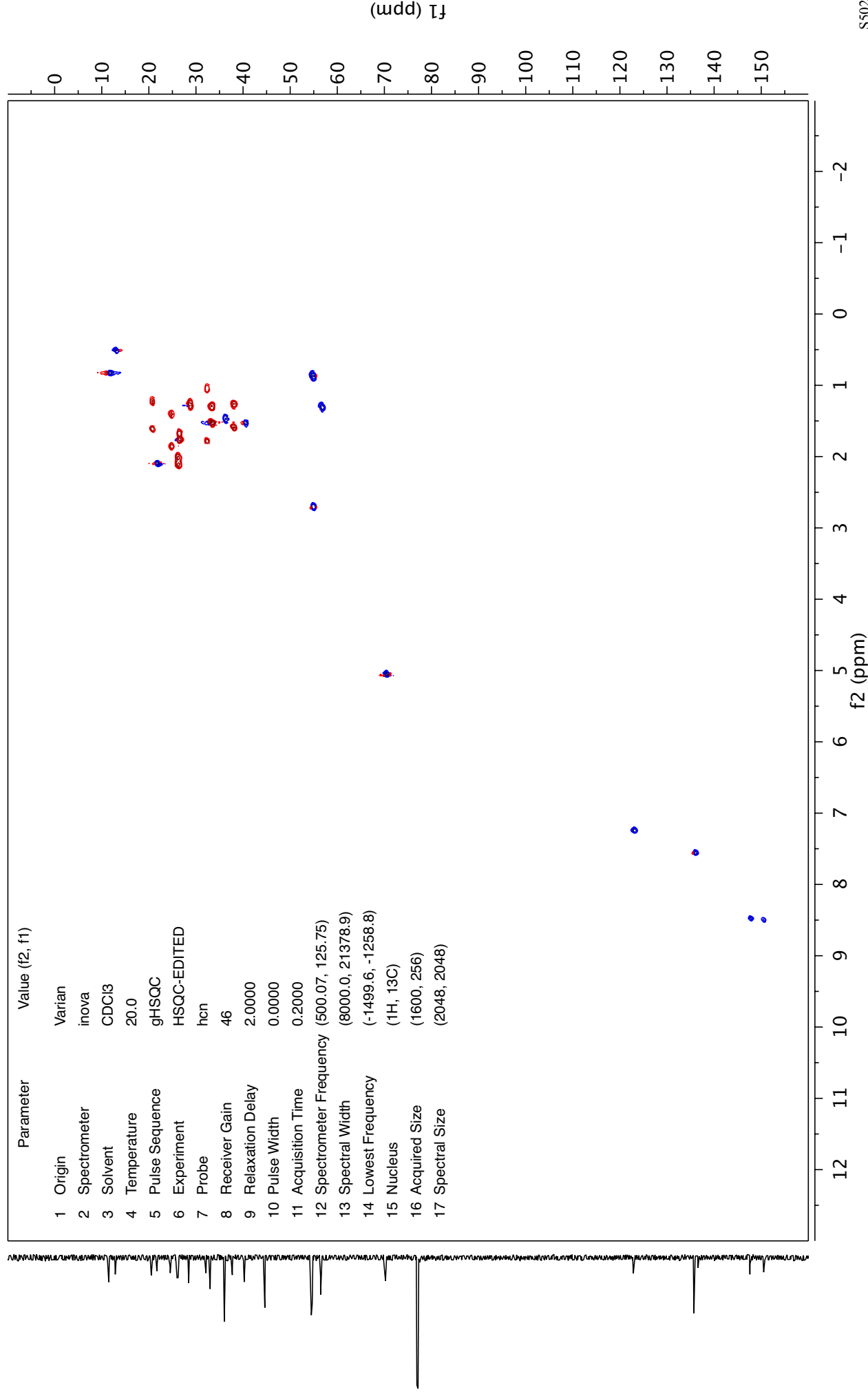
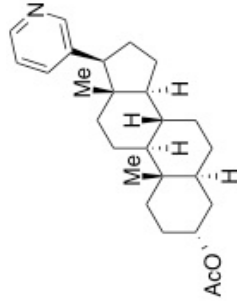


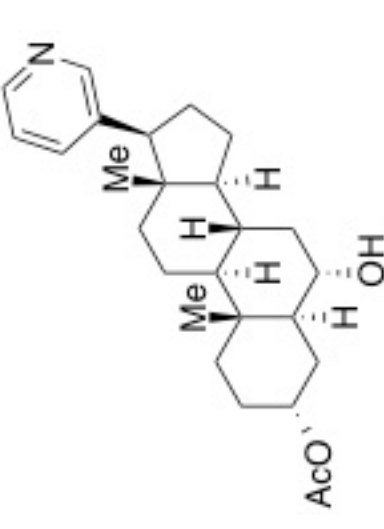
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUADG
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0240
Spectrometer Frequency	125.60
Spectral Width	32000.0
Lowest Frequency	-2201.7
Nucleus	¹³ C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



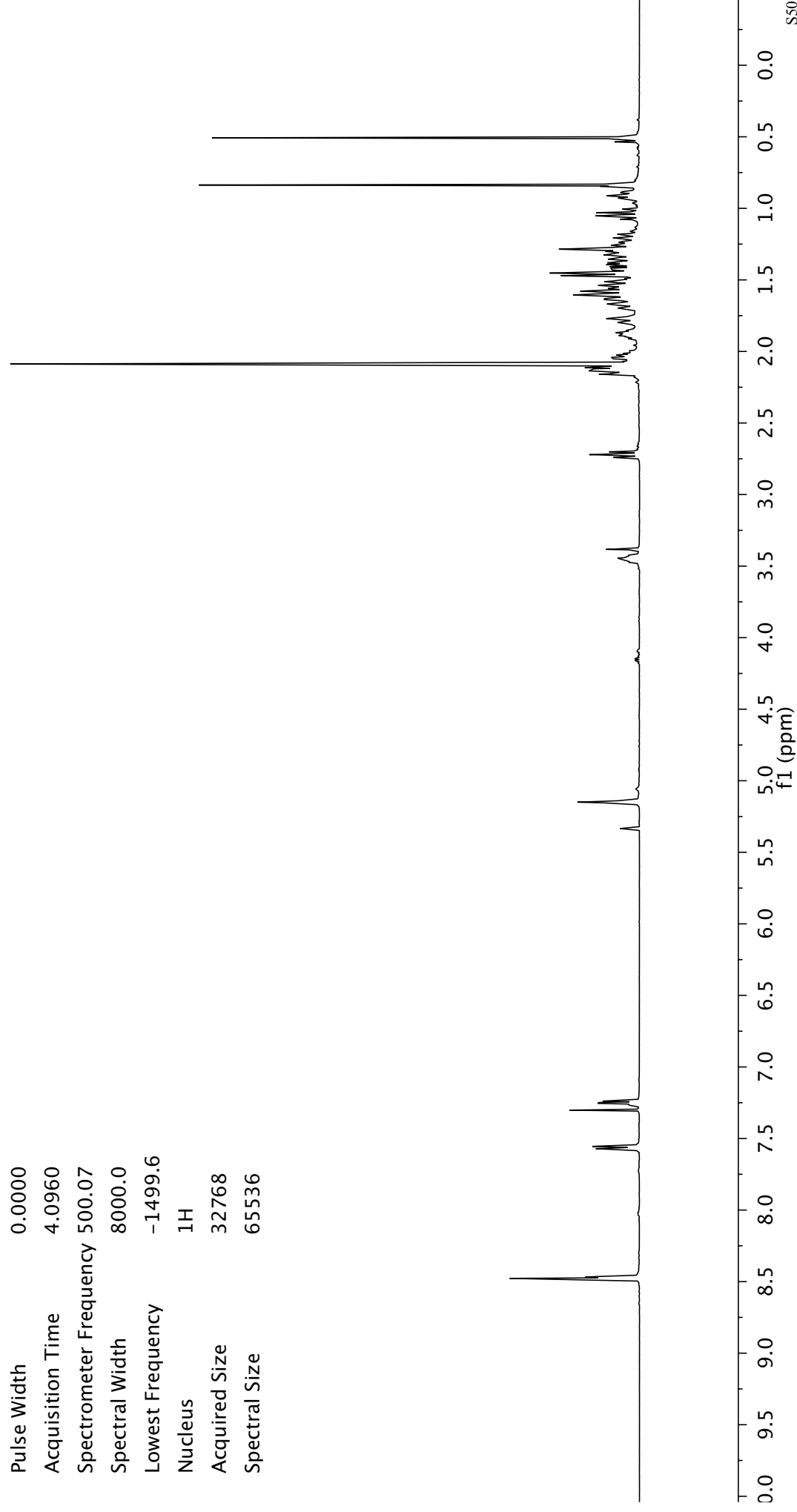


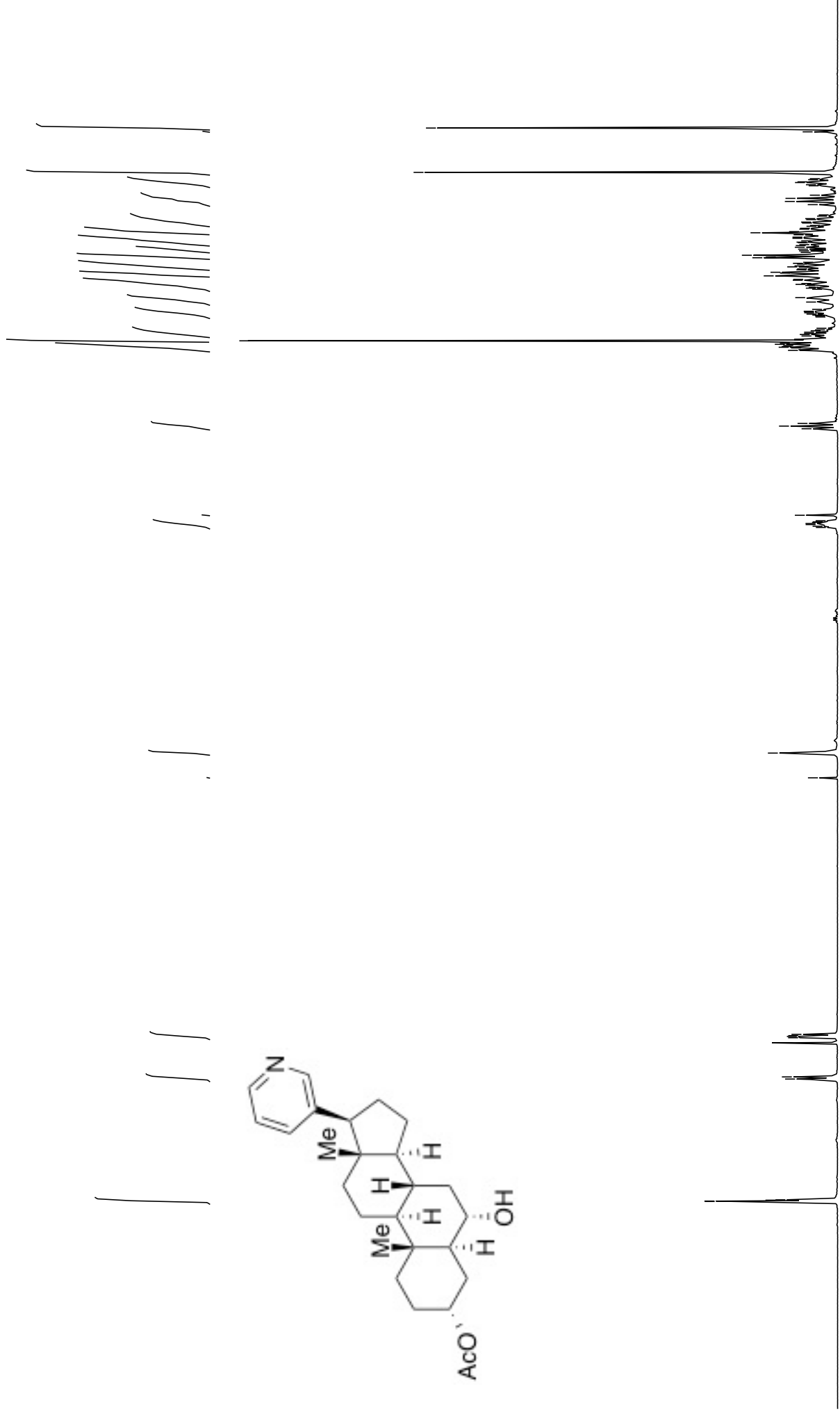
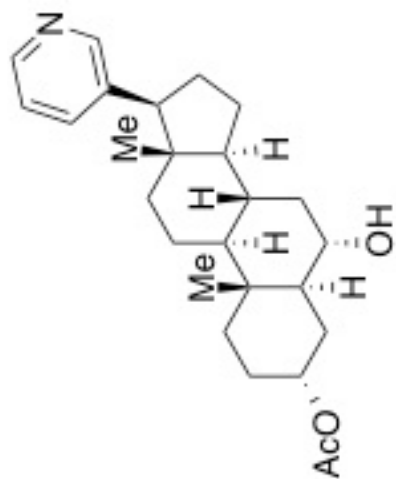
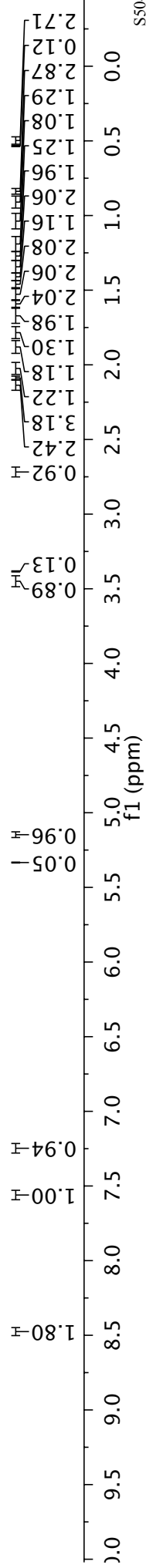


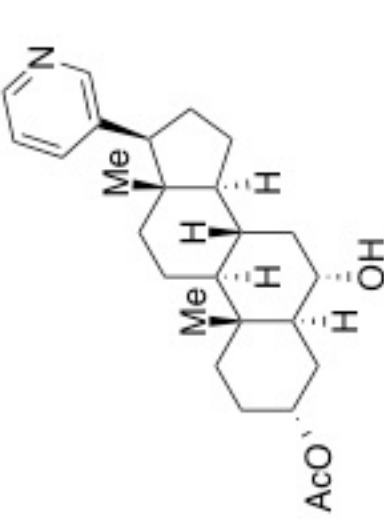




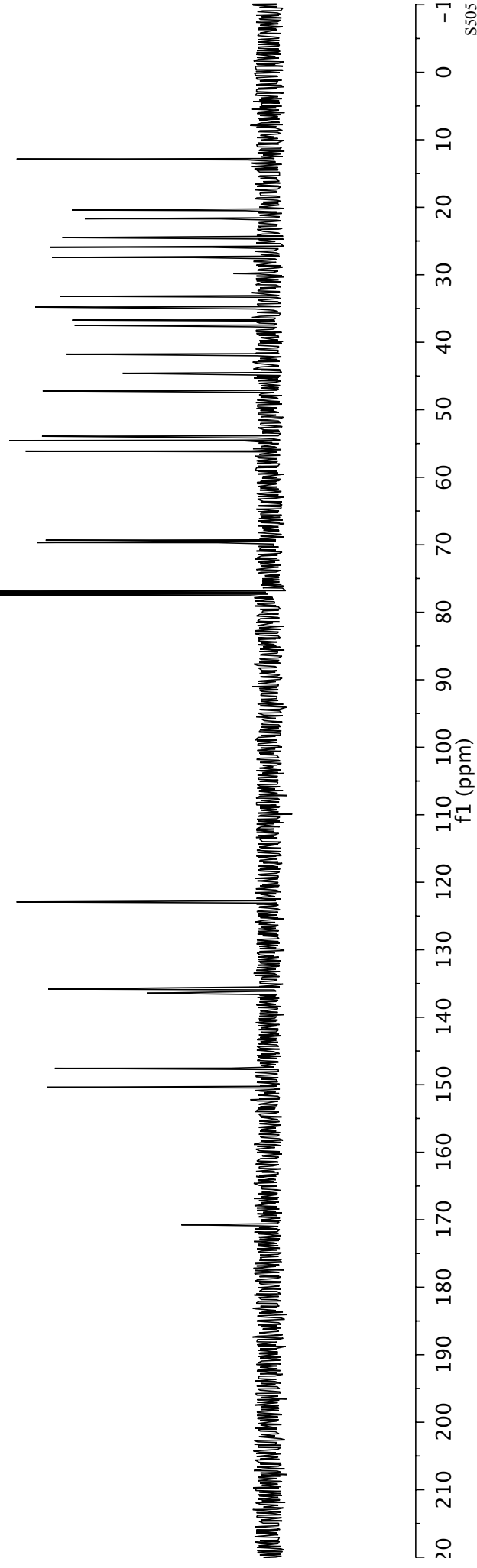
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	32
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1499.6
Nucleus	¹ H
Acquired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

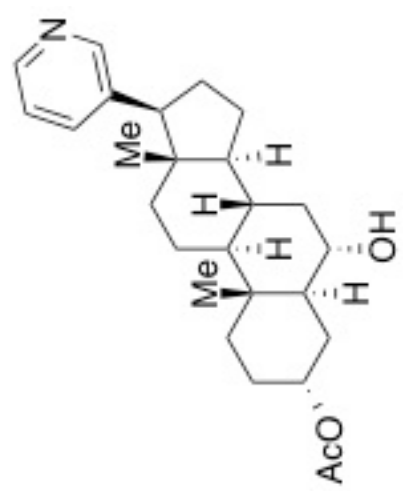
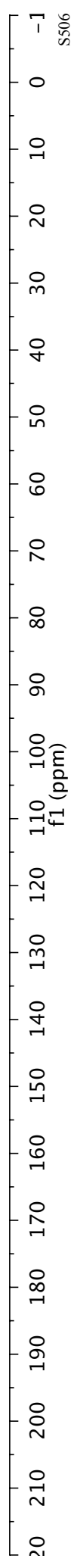




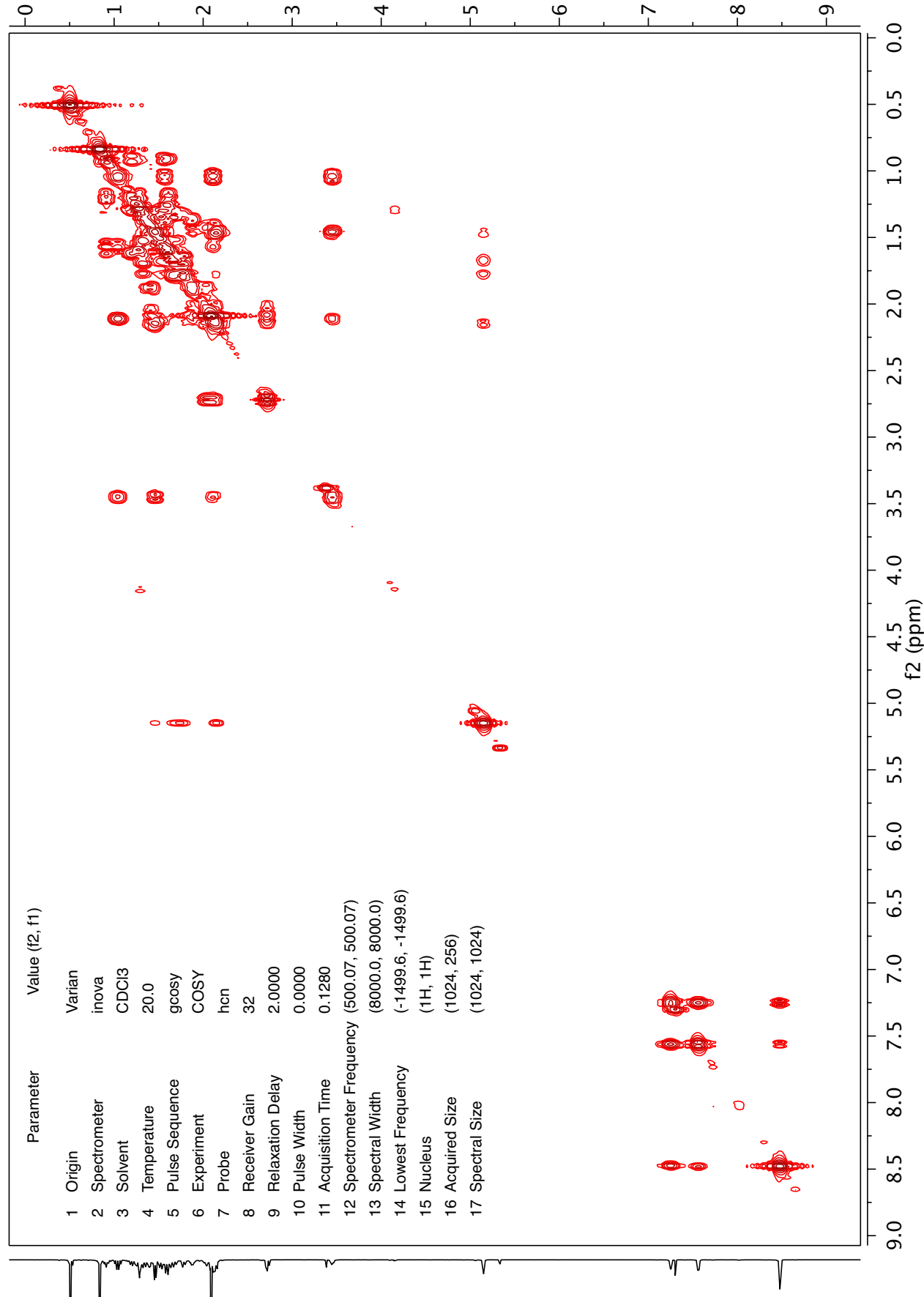
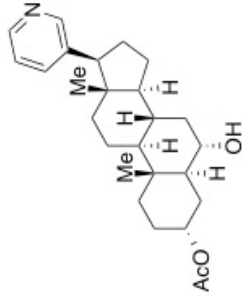


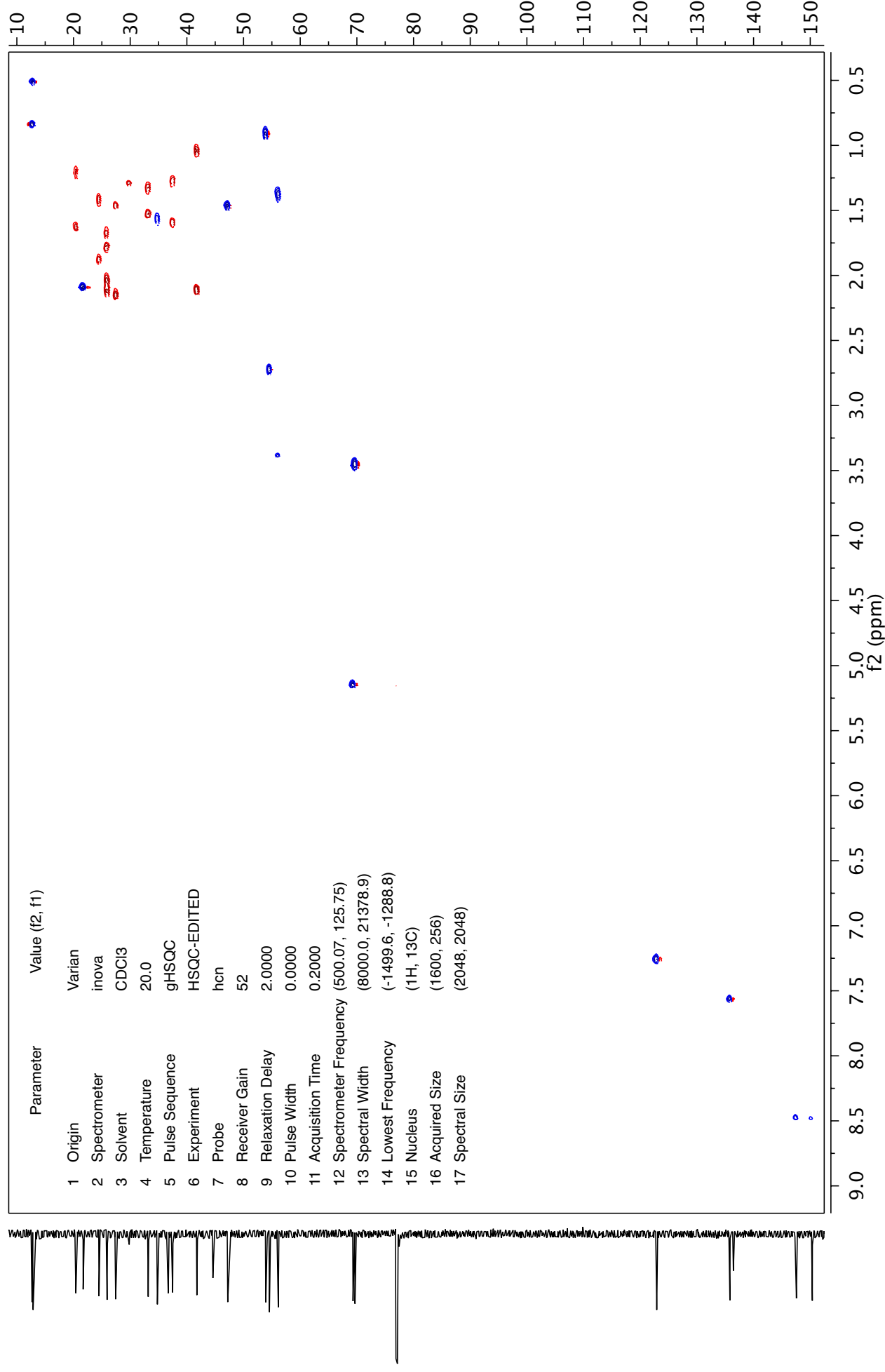
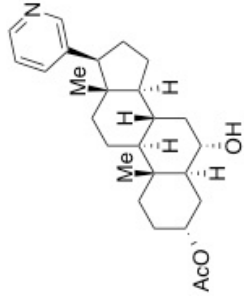
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	QUAD
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0863
Spectrometer Frequency	125.66
Spectral Width	30165.9
Lowest Frequency	-1274.8
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536



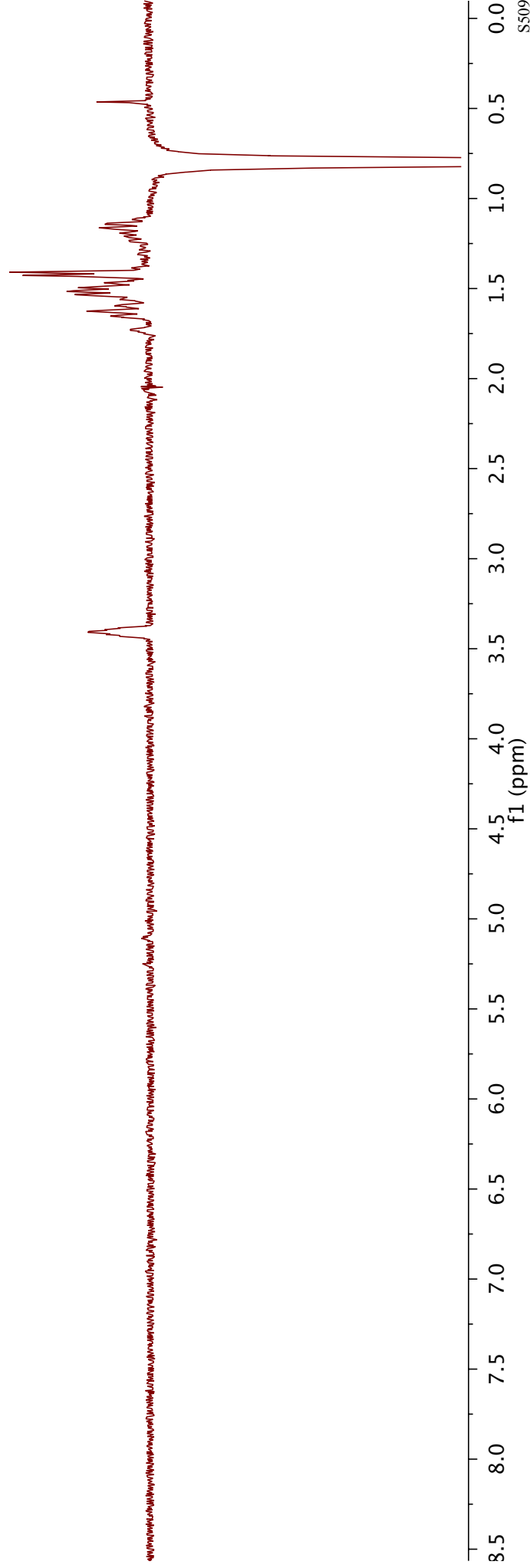
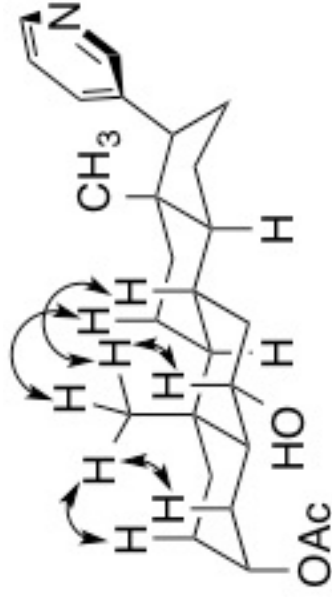


- 12.68
- 12.87
- 20.41
- 21.70
- 24.50
- 25.86
- 25.92
- 27.43
- 33.18
- 34.80
- 36.72
- 37.49
- 41.76
- 44.59
- 47.21
- 53.93
- 54.57
- 56.13
- 69.32
- 69.67
- 76.90 CDCl₃
- 77.16 CDCl₃
- 77.41 CDCl₃
- 122.92
- 135.82
- 136.44
- 147.56
- 150.37
- 170.75

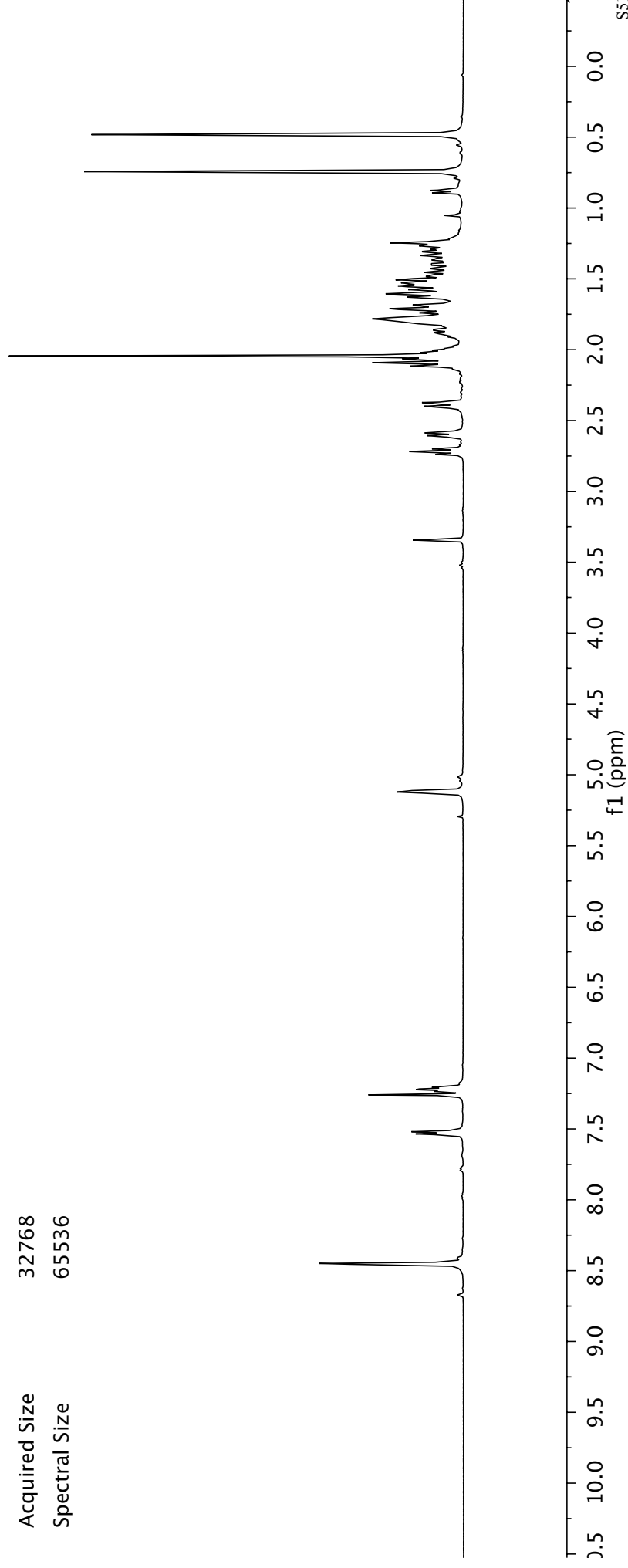
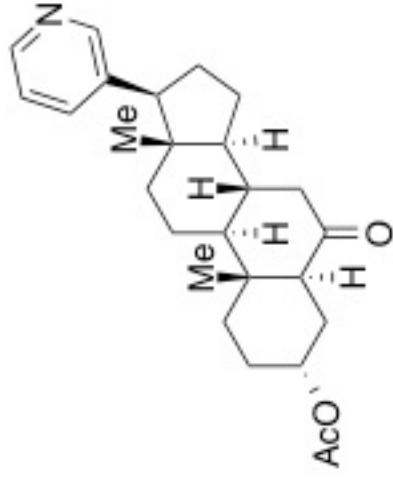


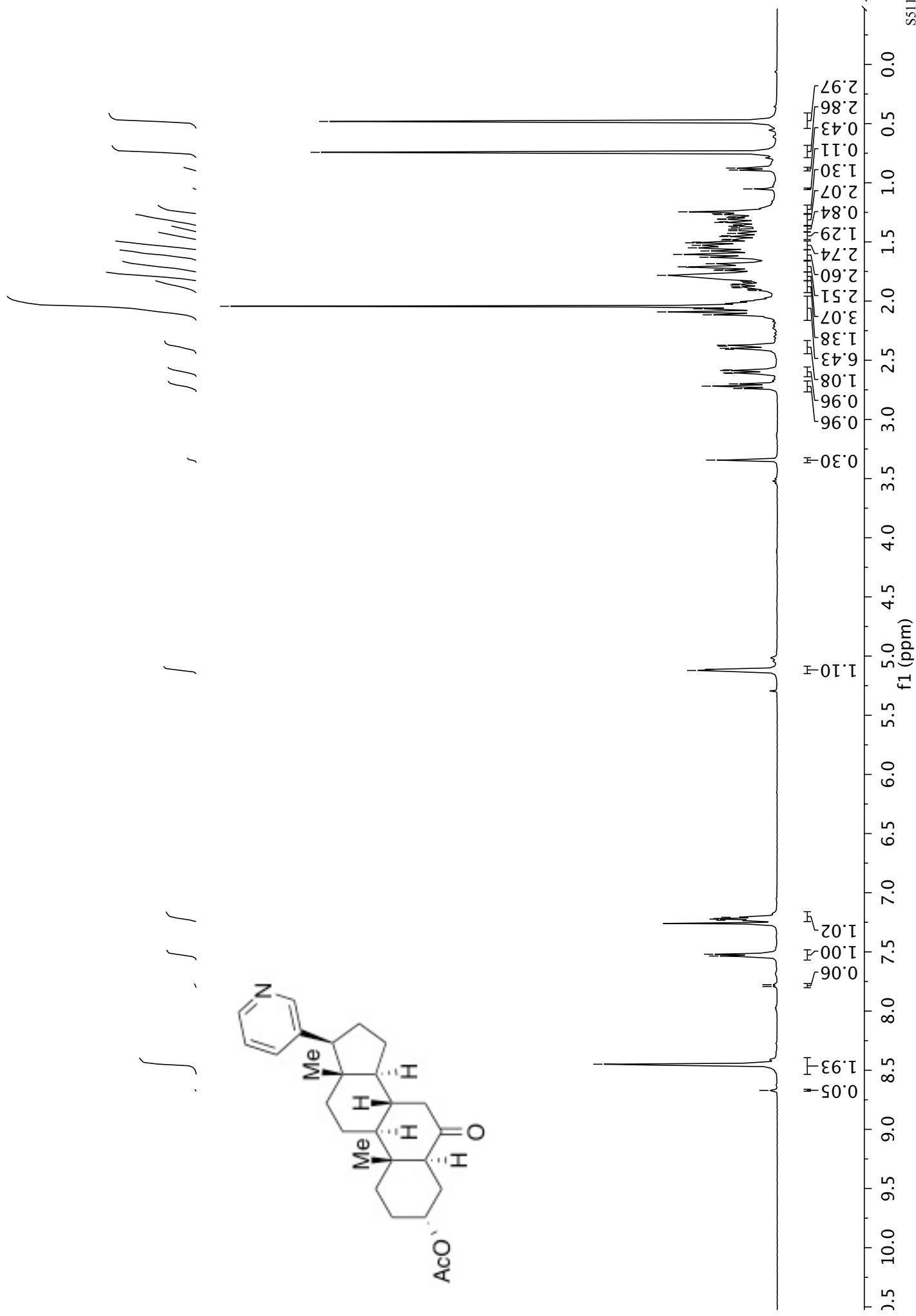


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	NOESY1D
Experiment	1D-NOESY
Probe	hcn
Receiver Gain	44
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1520.9
Nucleus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

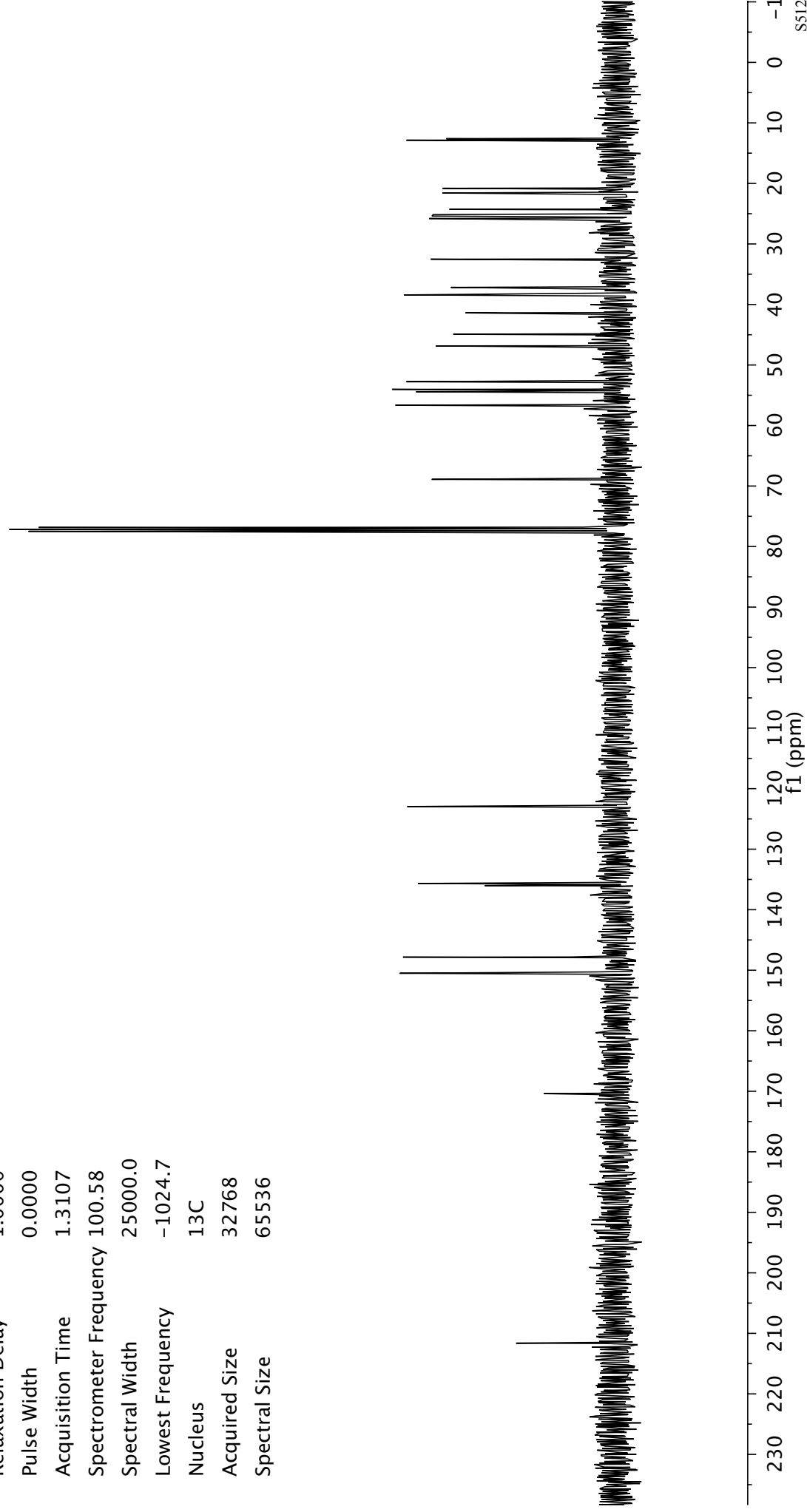
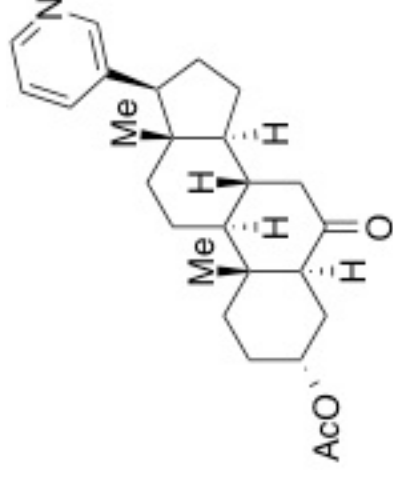


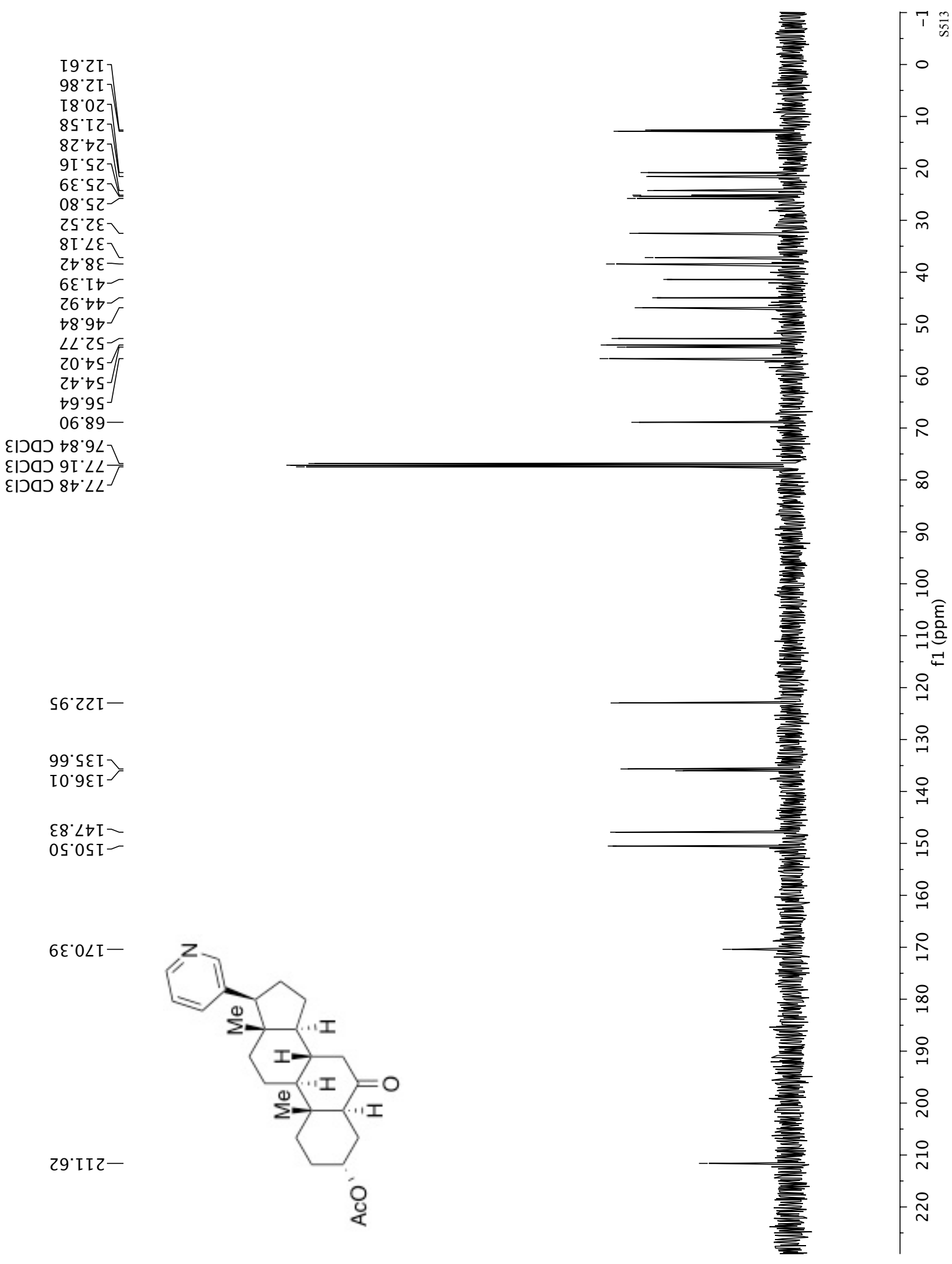
Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl ₃
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	hcn
Receiver Gain	44
Relaxation Delay	0.0000
Pulse Width	0.0000
Acquisition Time	4.0960
Spectrometer Frequency	500.07
Spectral Width	8000.0
Lowest Frequency	-1520.4
Nucleus	¹ H
Acquired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

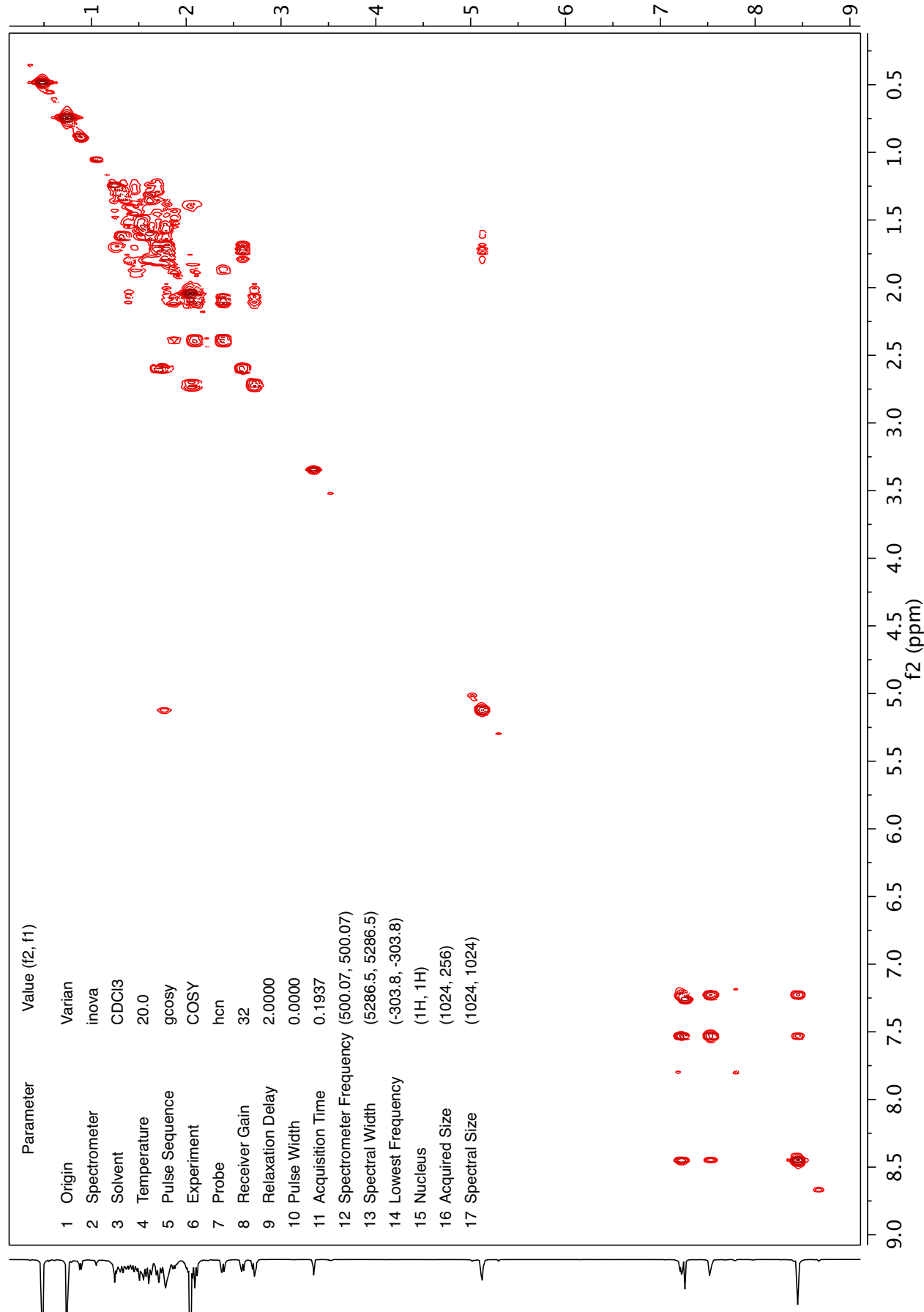
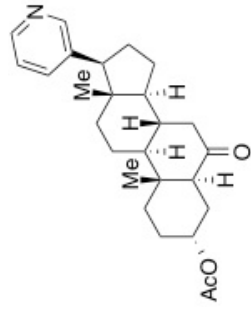


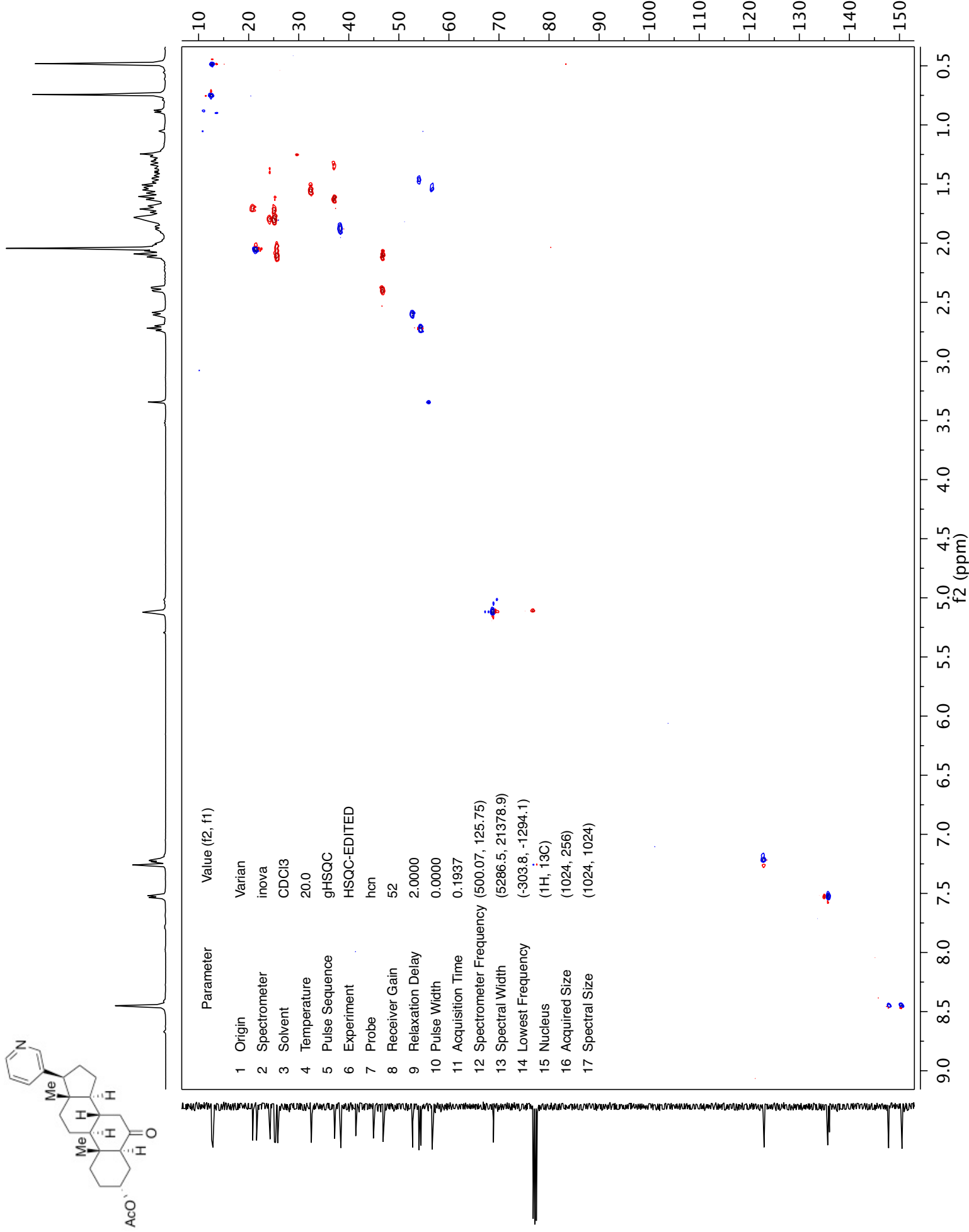
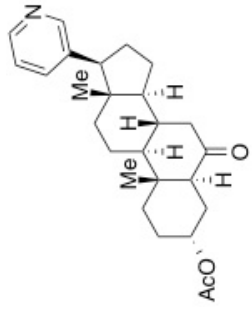


Parameter	Value
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	20.0
Pulse Sequence	s2pul
Experiment	1D
Probe	quad94
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3107
Spectrometer Frequency	100.58
Spectral Width	25000.0
Lowest Frequency	-1024.7
Nucleus	¹³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



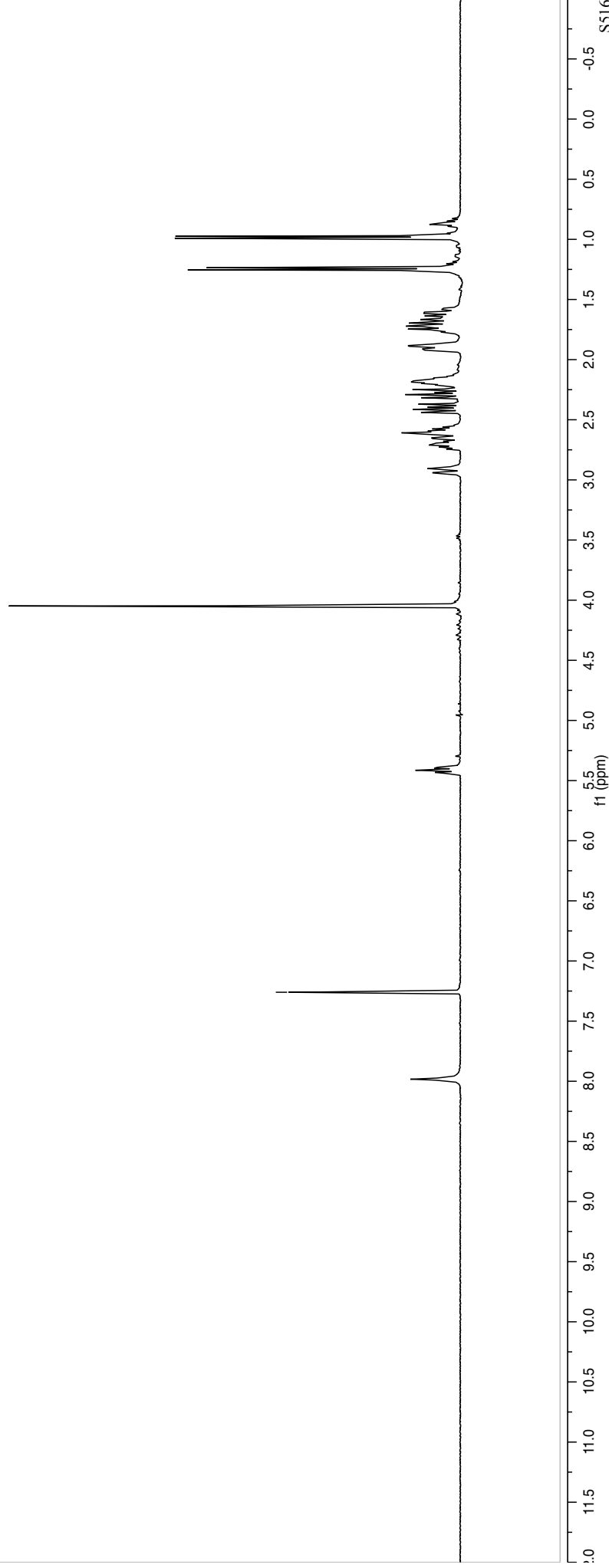
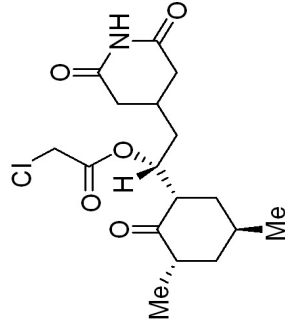


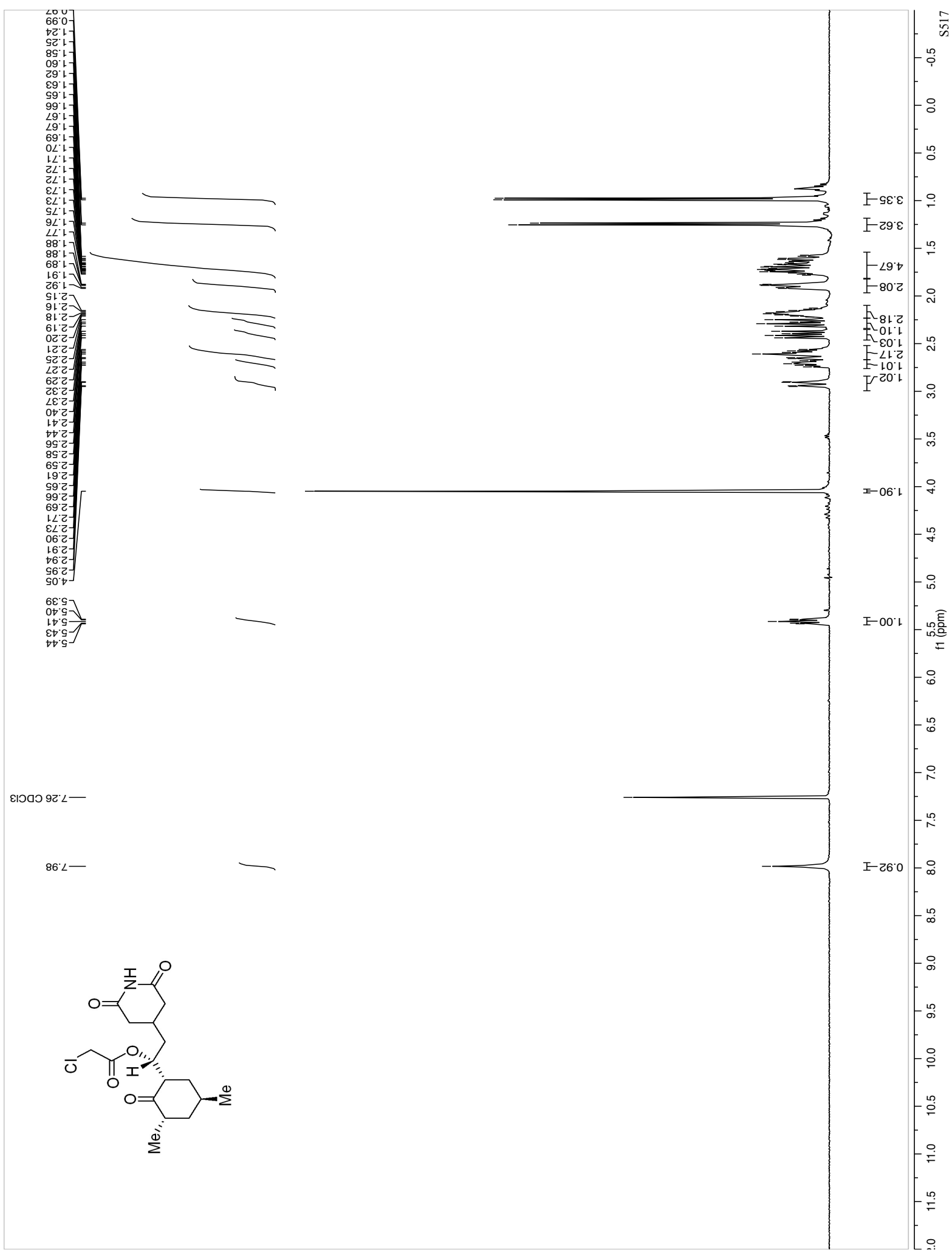




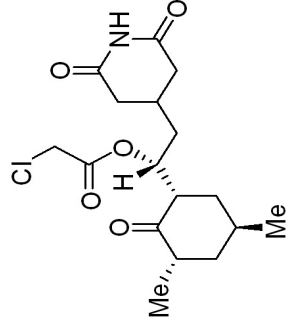
7.3 CDCl3

Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl3
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	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	1H
17 Acquired Size	32768
18 Spectral Size	65536

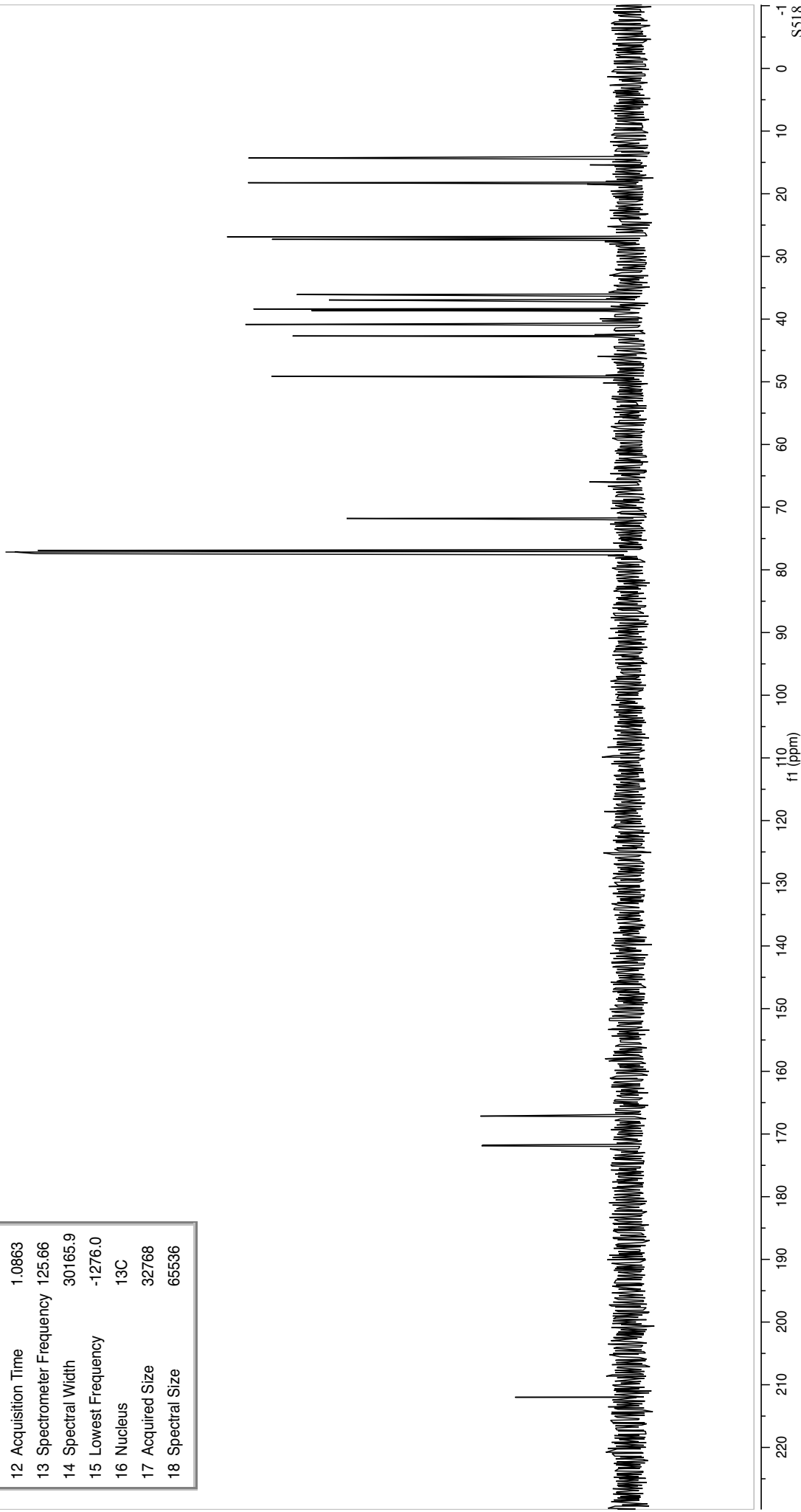


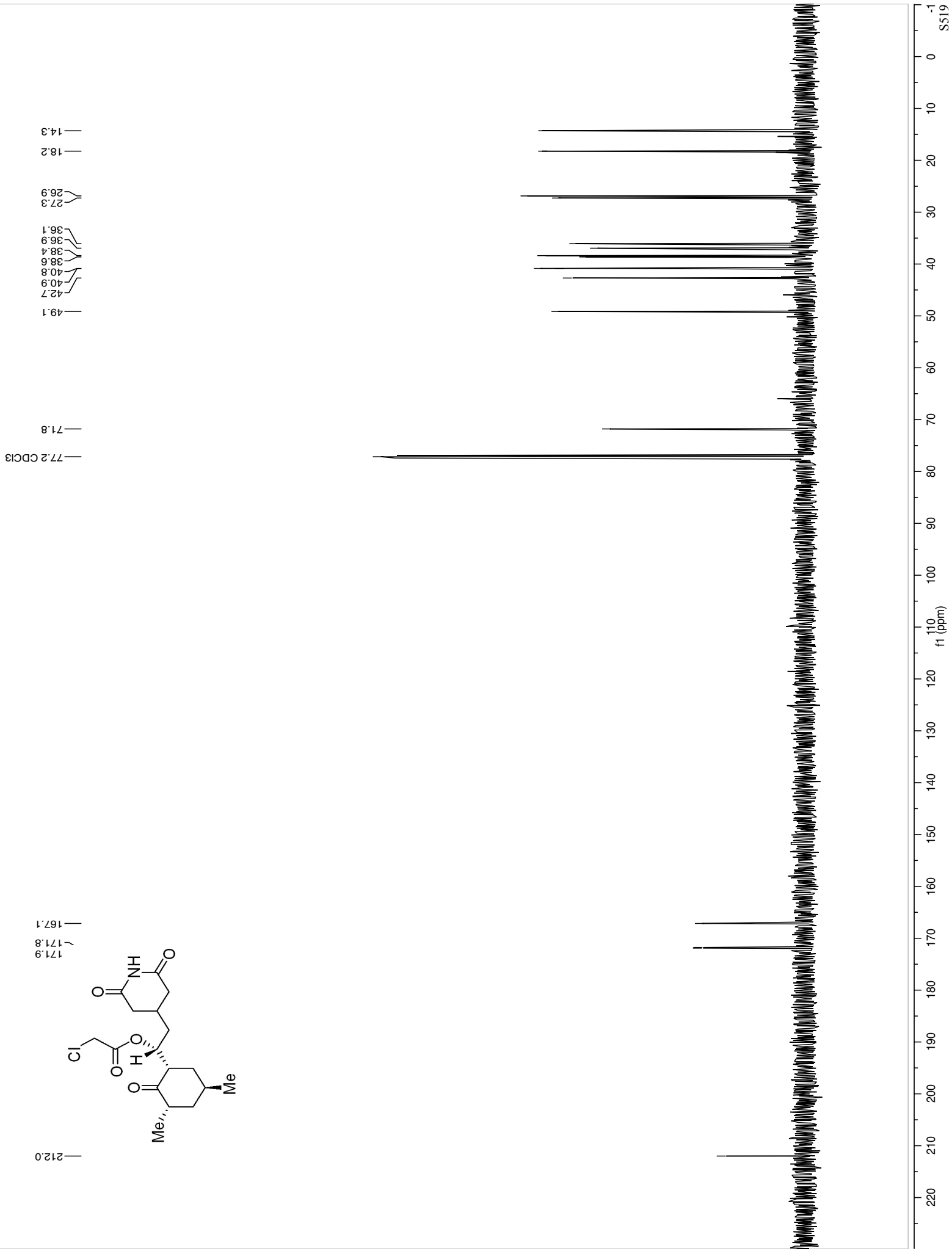


Parameter	Value
1 Origin	Varian
2 Spectrometer	inova
3 Solvent	CDCl ₃
4 Temperature	20.0
5 Pulse Sequence	s2pul
6 Experiment	1D
7 Probe	QUAD
8 Number of Scans	176
9 Receiver Gain	60
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.0863
13 Spectrometer Frequency	125.66
14 Spectral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



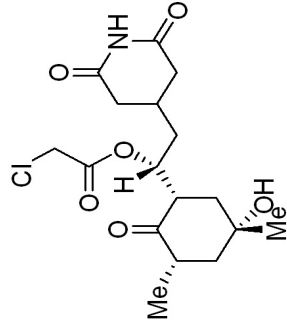
— 77.2 CDCl₃



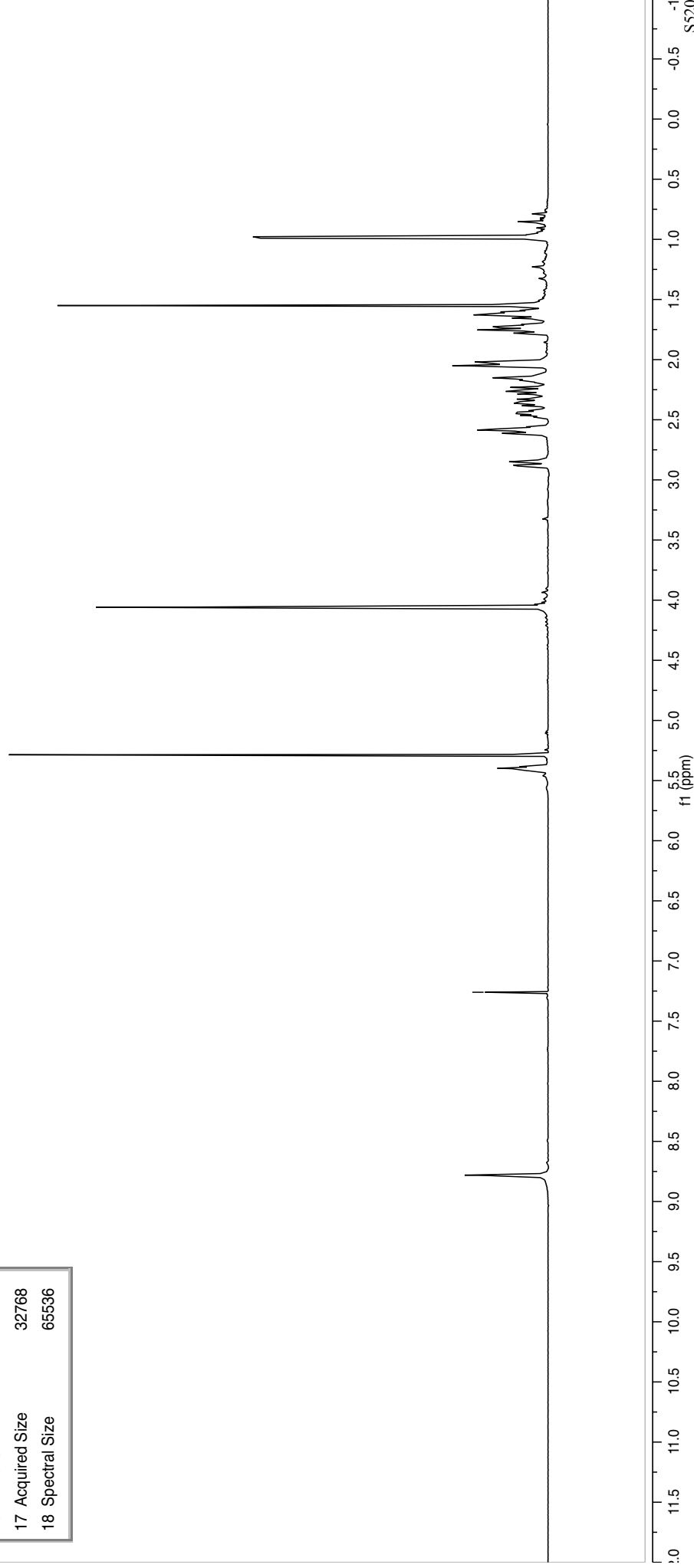


7.3 CDCl₃

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	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

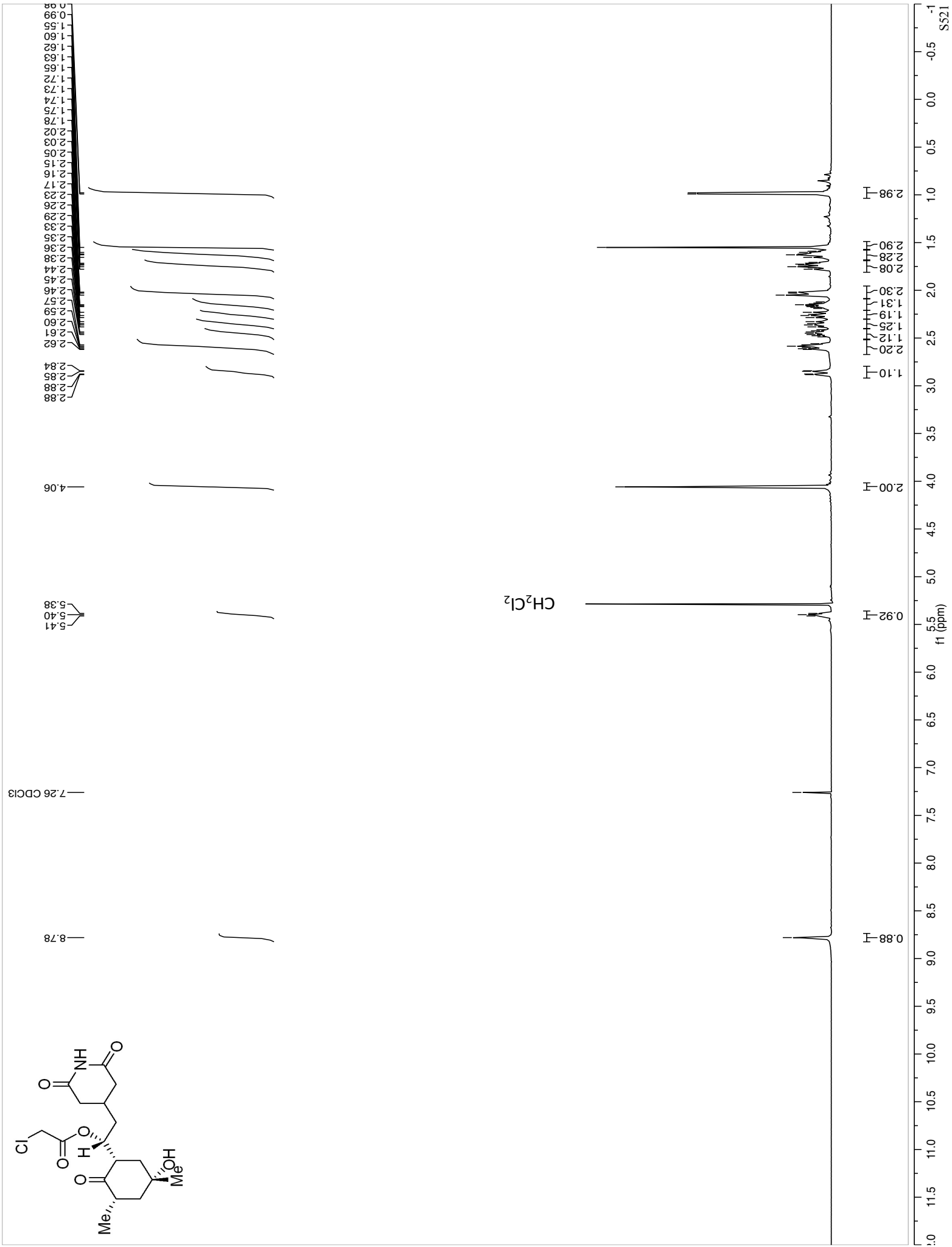


CH₂Cl₂

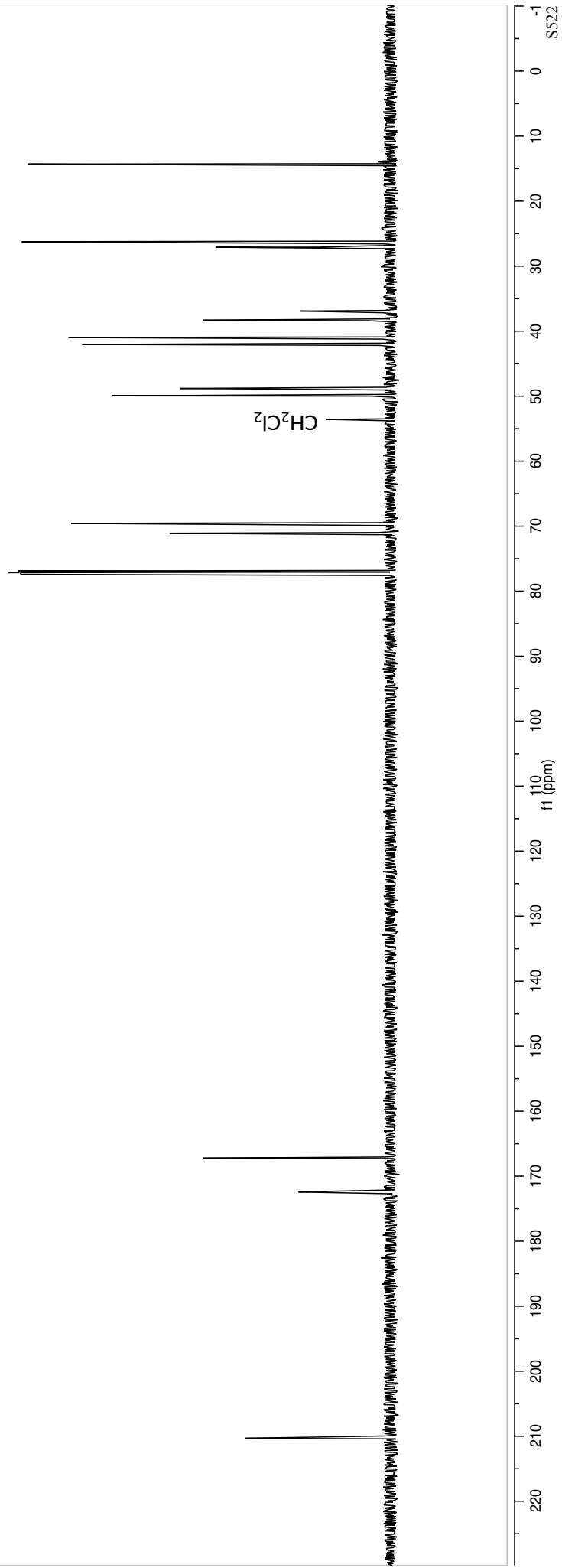
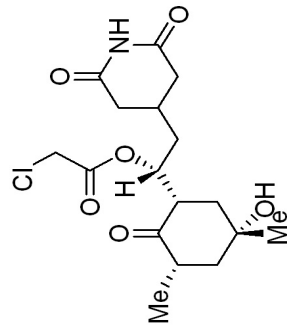


f1 (ppm)

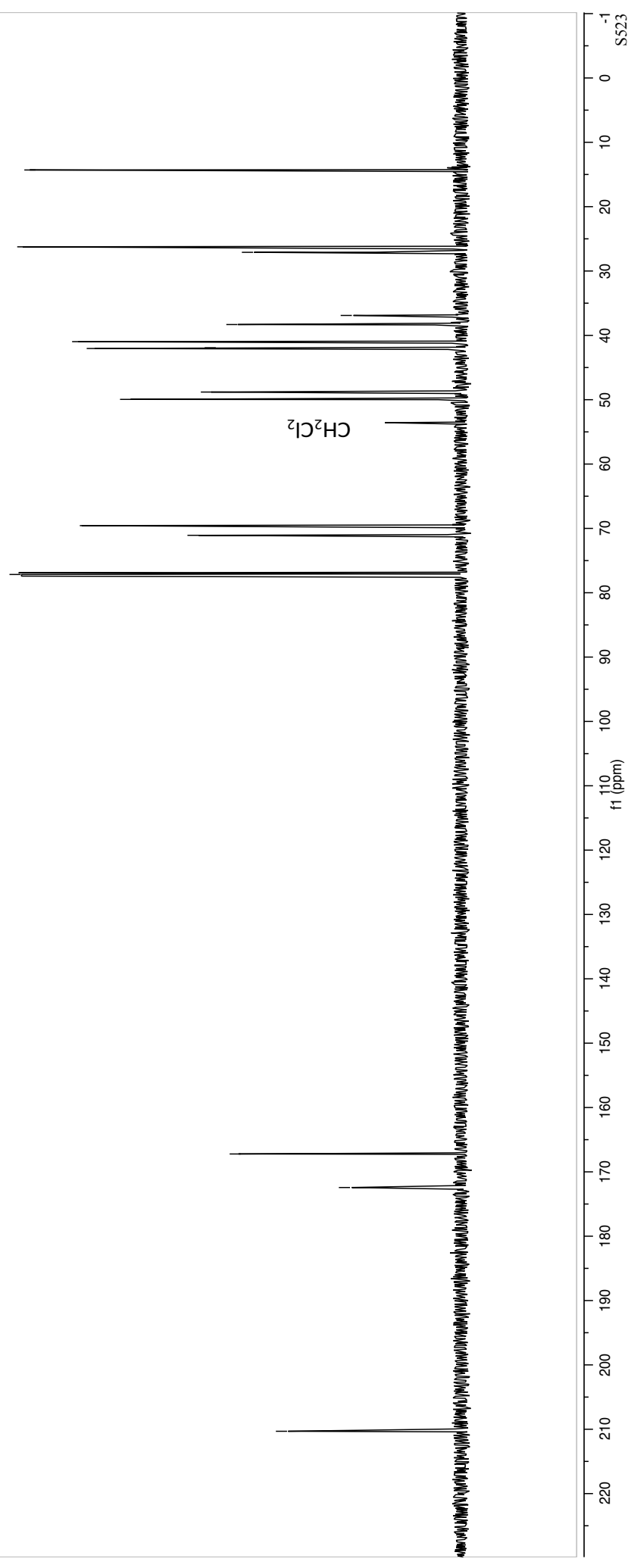
S520



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	¹³ C
17 Acquired Size	32768
18 Spectral Size	65536



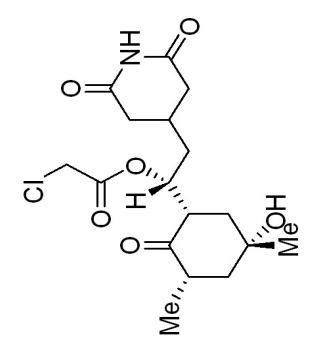
77.2 CDCl3



CH₂Cl₂

Chemical shift values (ppm):

- 14.3
- 26.2
- 27.1
- 36.9
- 38.3
- 41.0
- 41.9
- 42.0
- 48.8
- 50.0
- 69.6
- 71.1
- 77.2 CDCl₃



Chemical shift values (ppm):

- 167.2
- 172.4
- 210.3