

## Supporting Information

# **An Unusual Wittig Reaction with Sugar Derivatives: Exclusive Formation of a 4-Deoxy Analogue of $\alpha$ -Galactosyl Ceramide**

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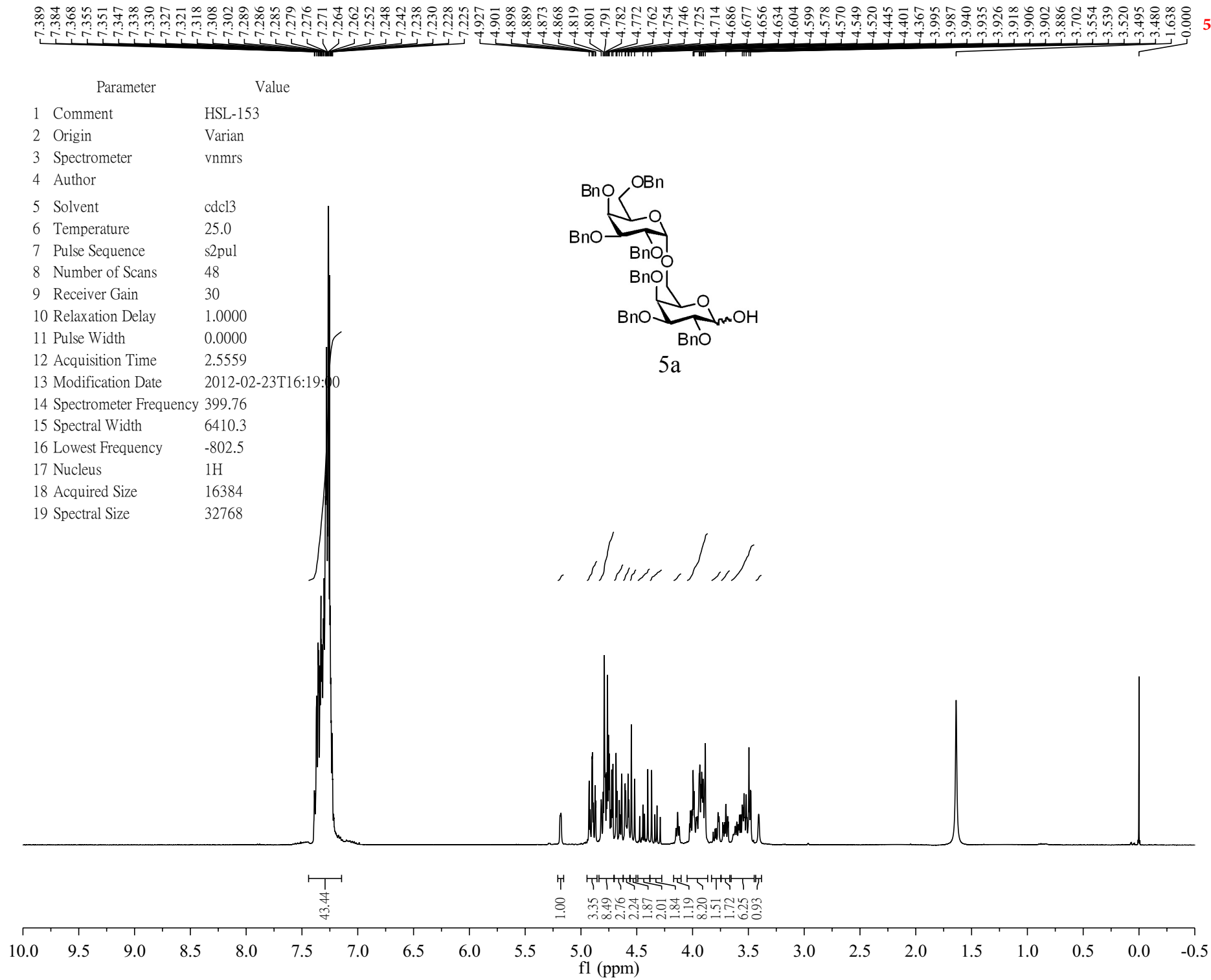
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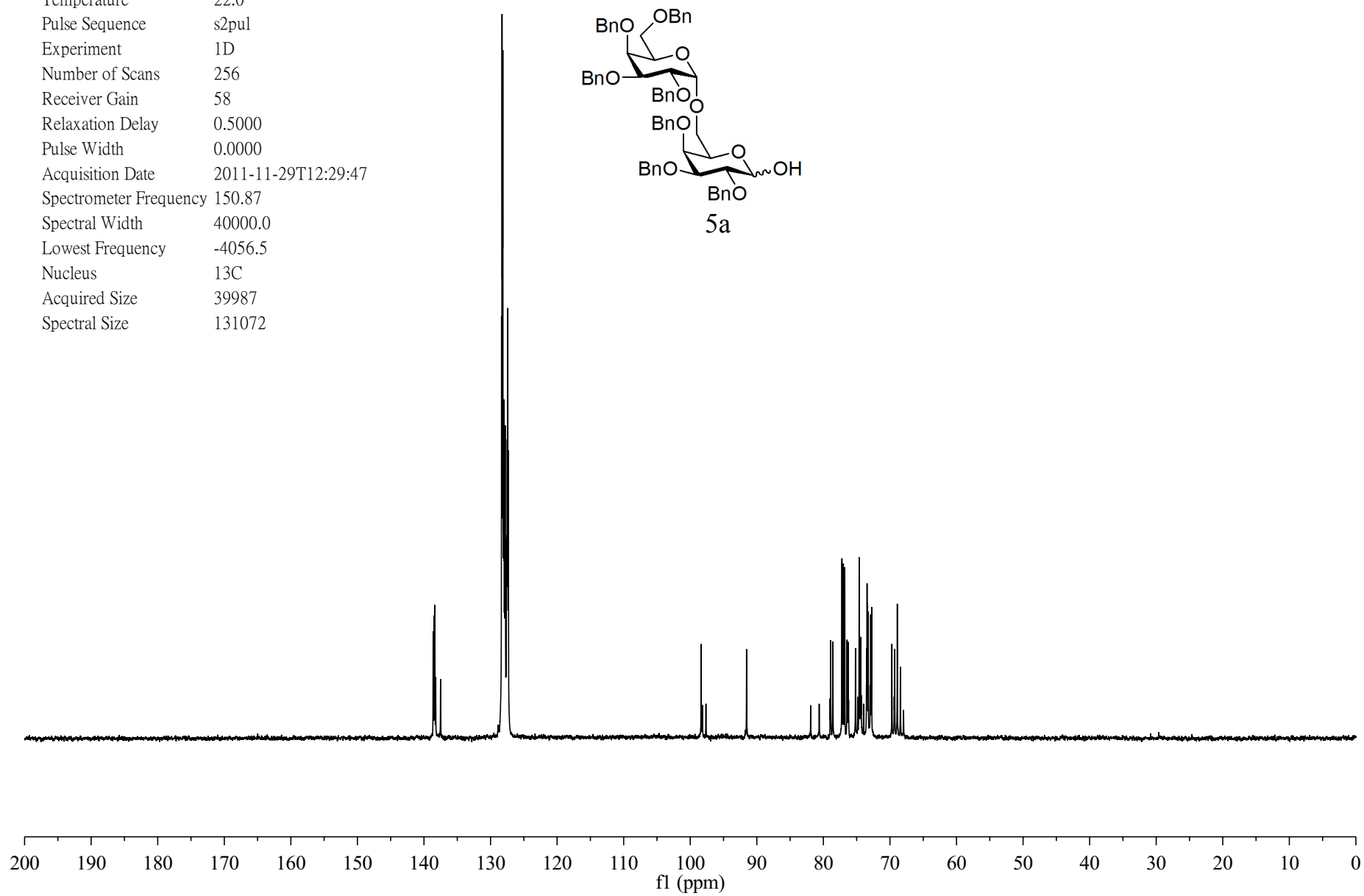
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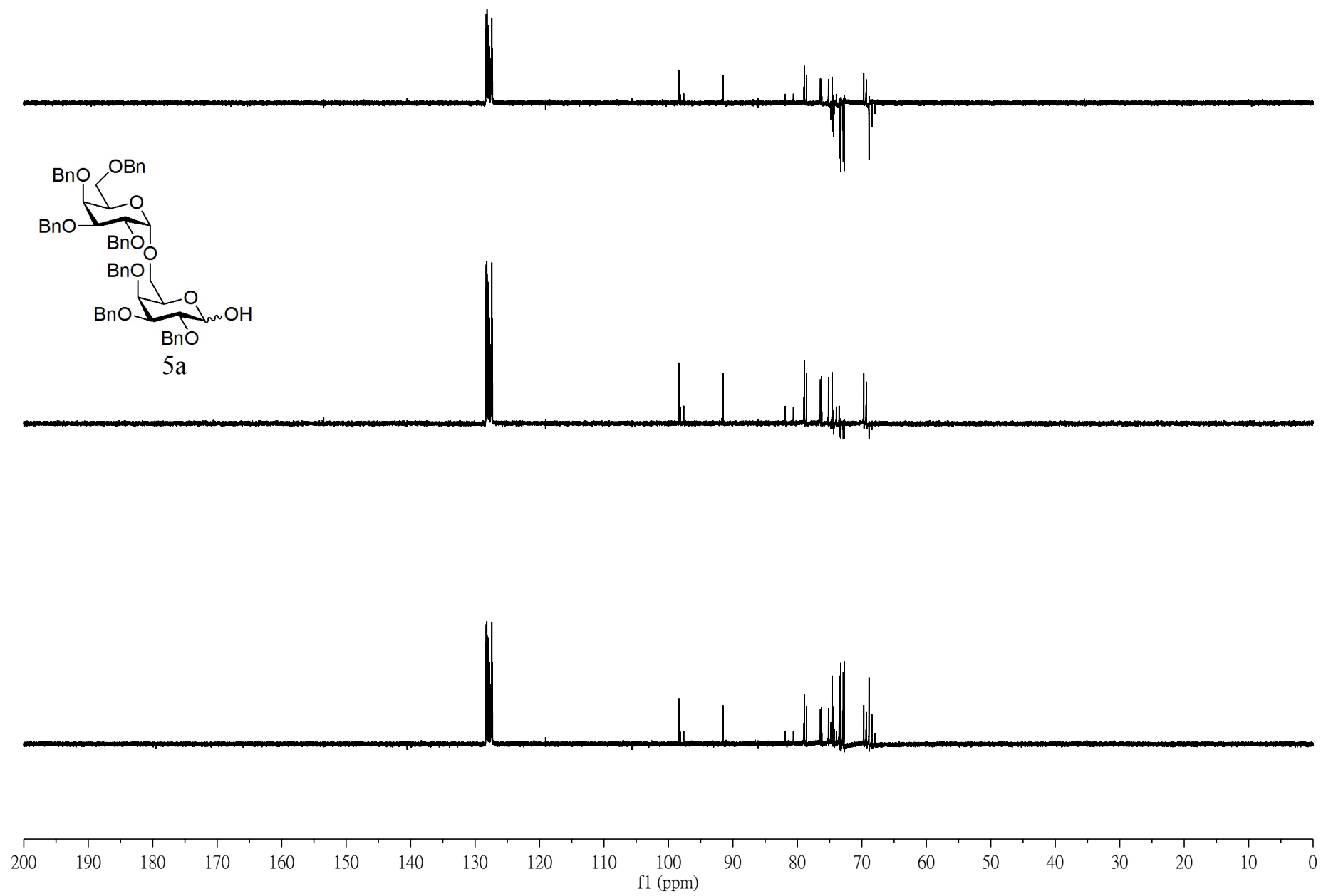
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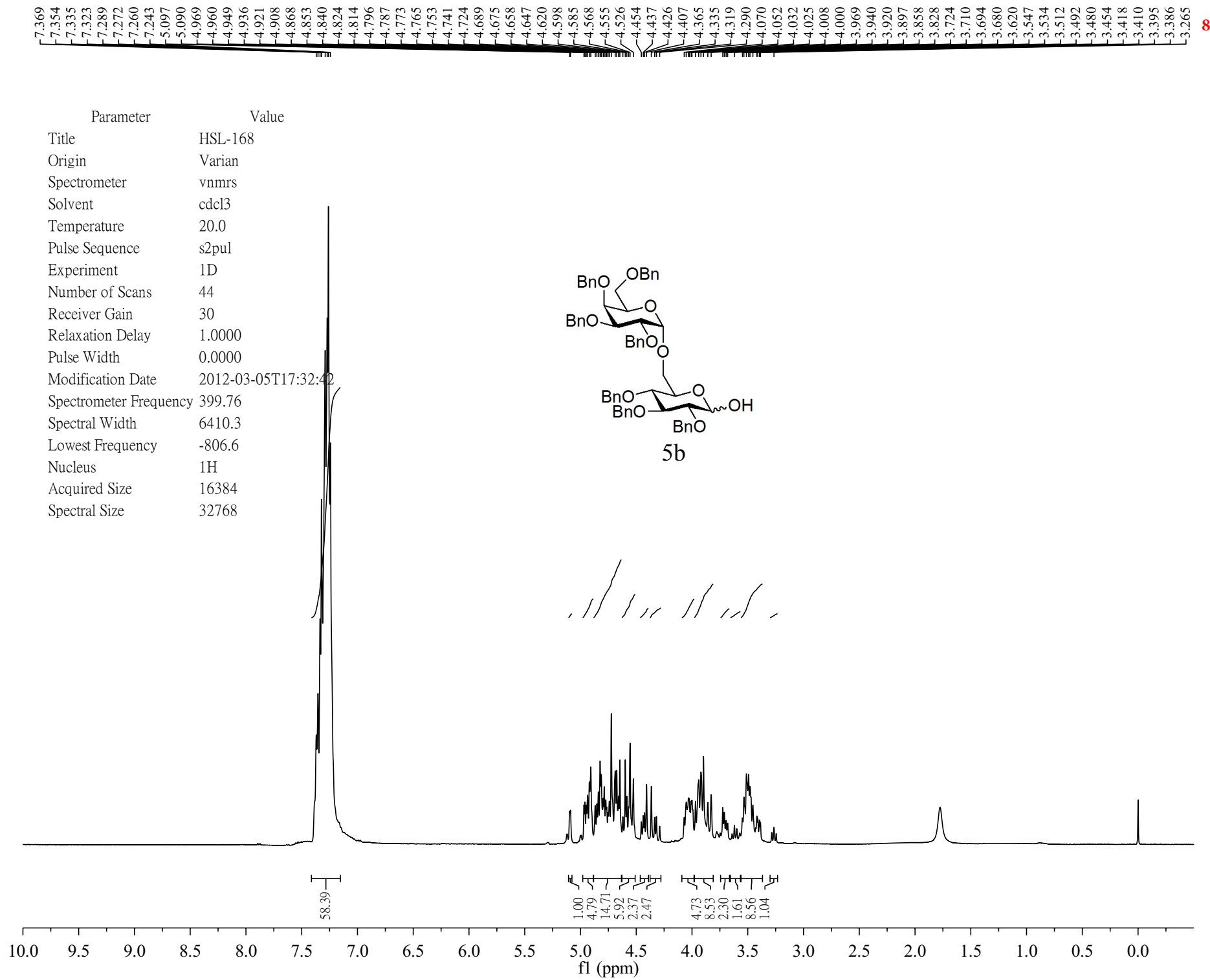
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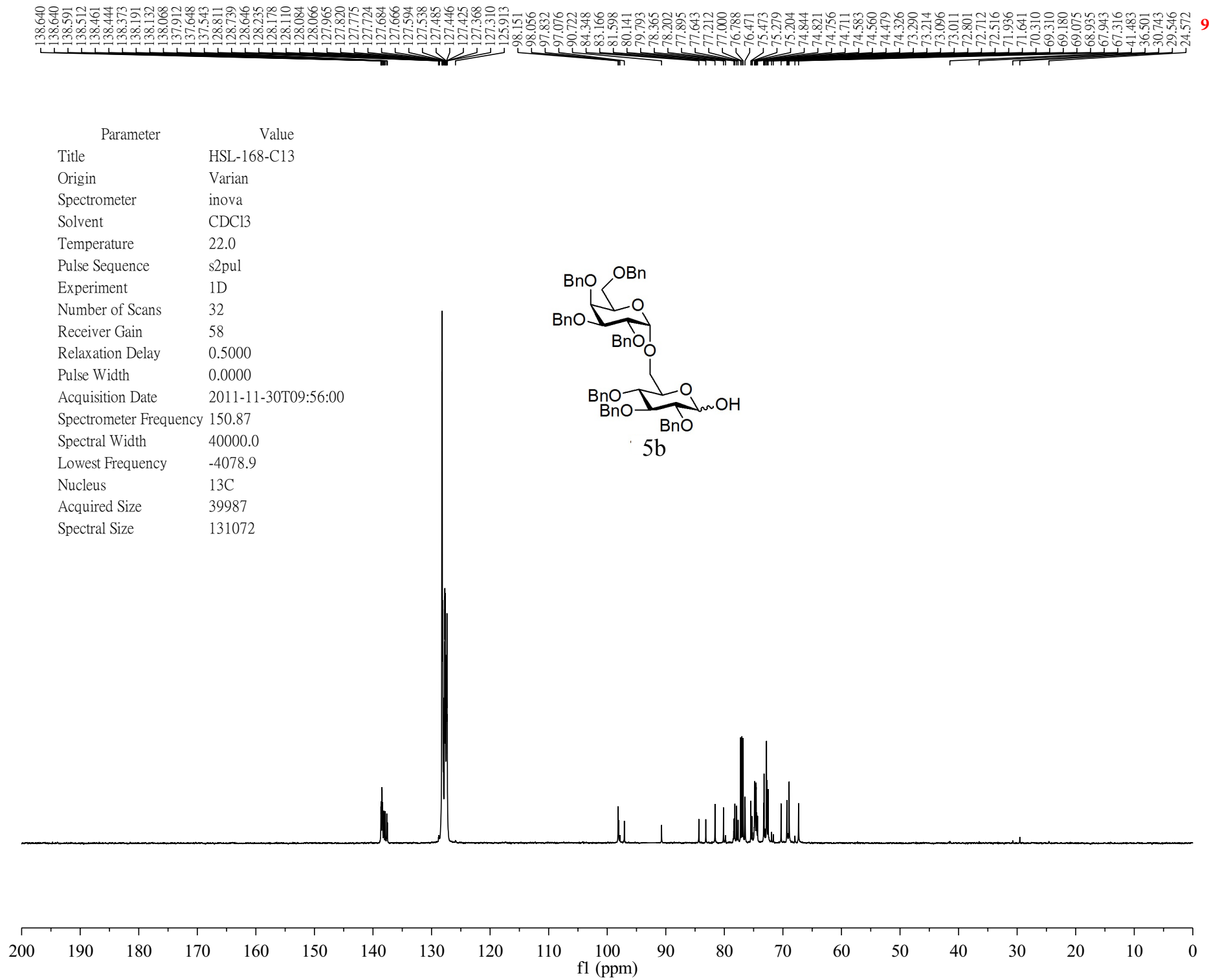
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Solvent	CDC13
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Receiver Gain	58
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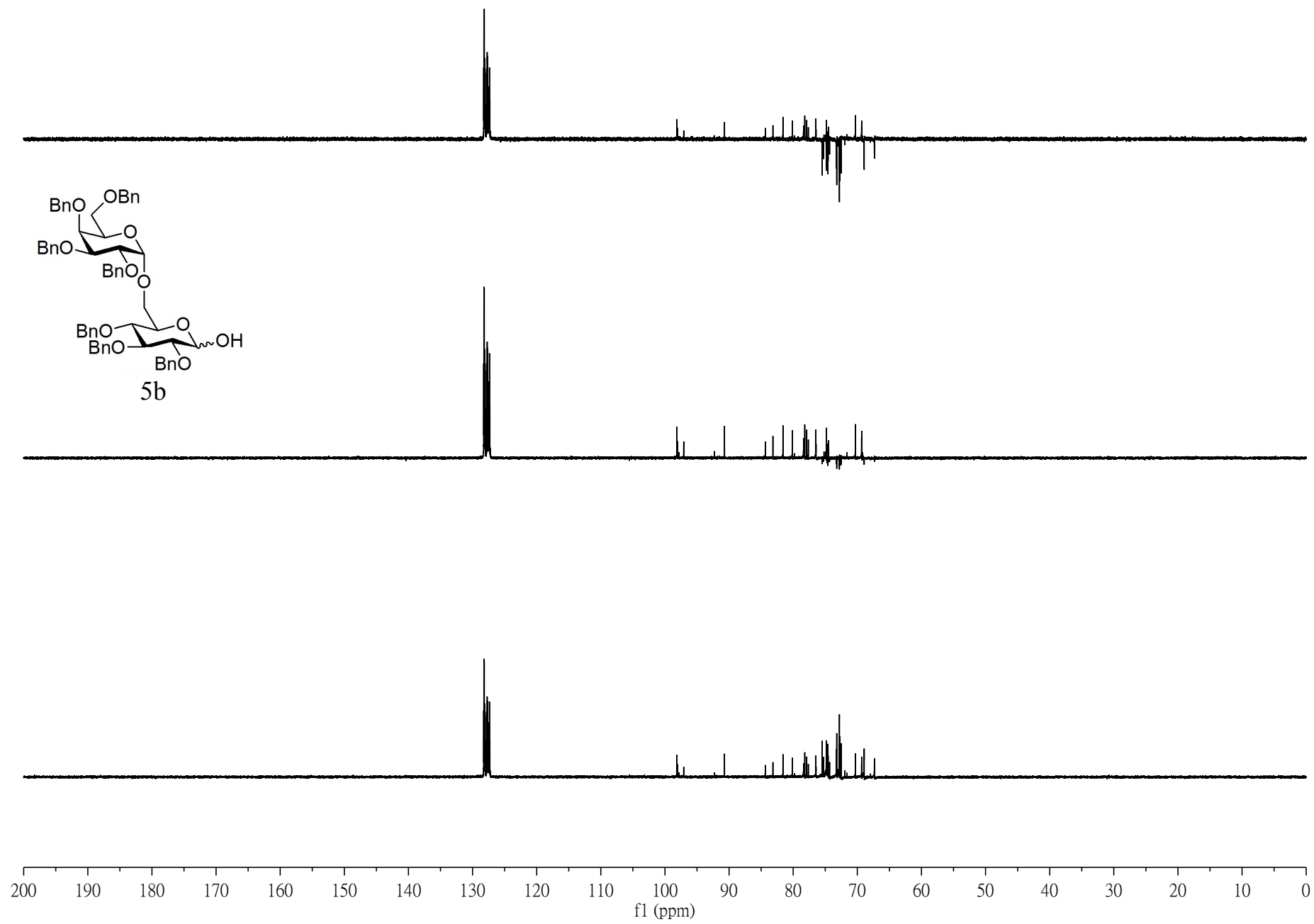




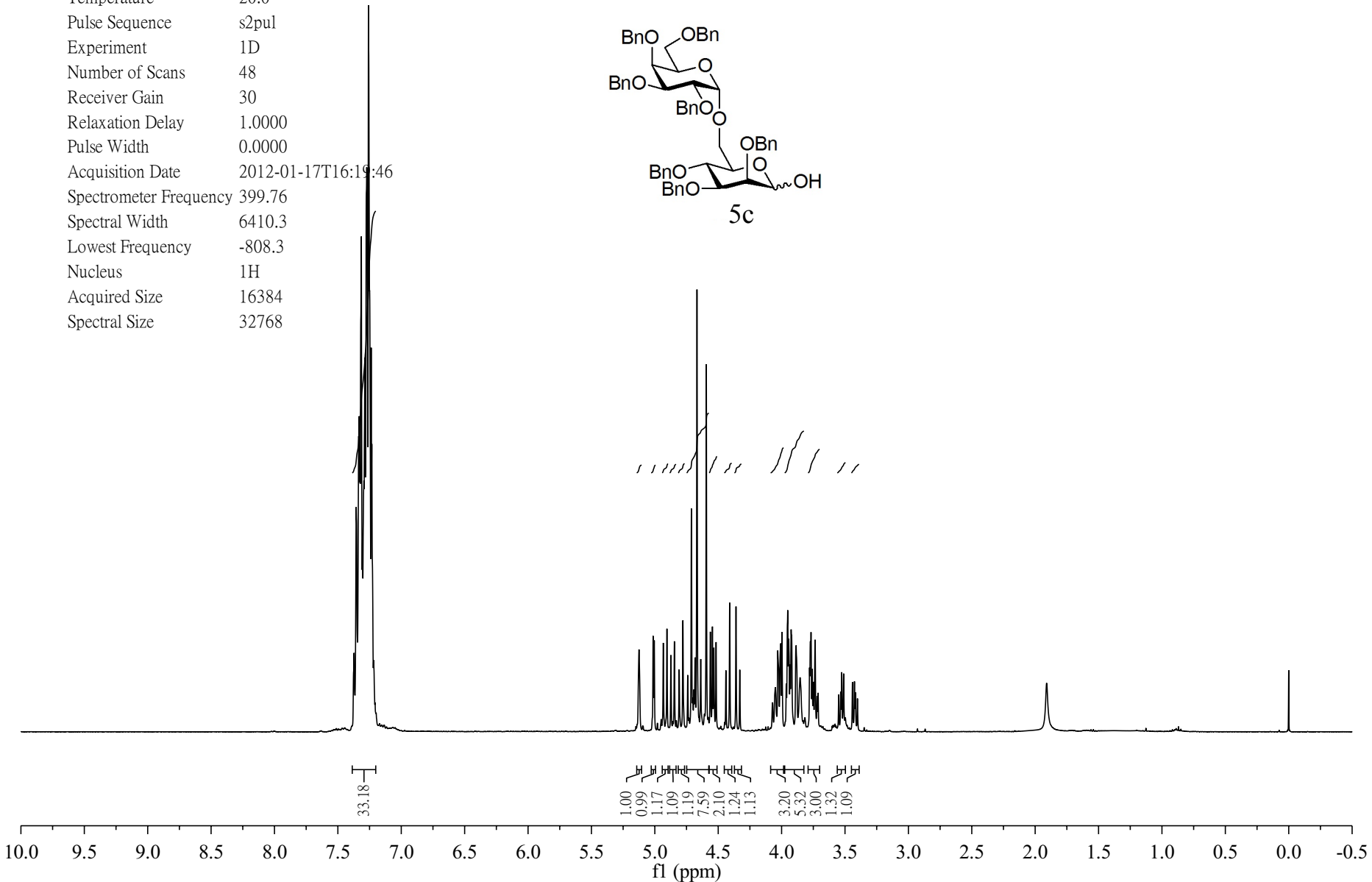






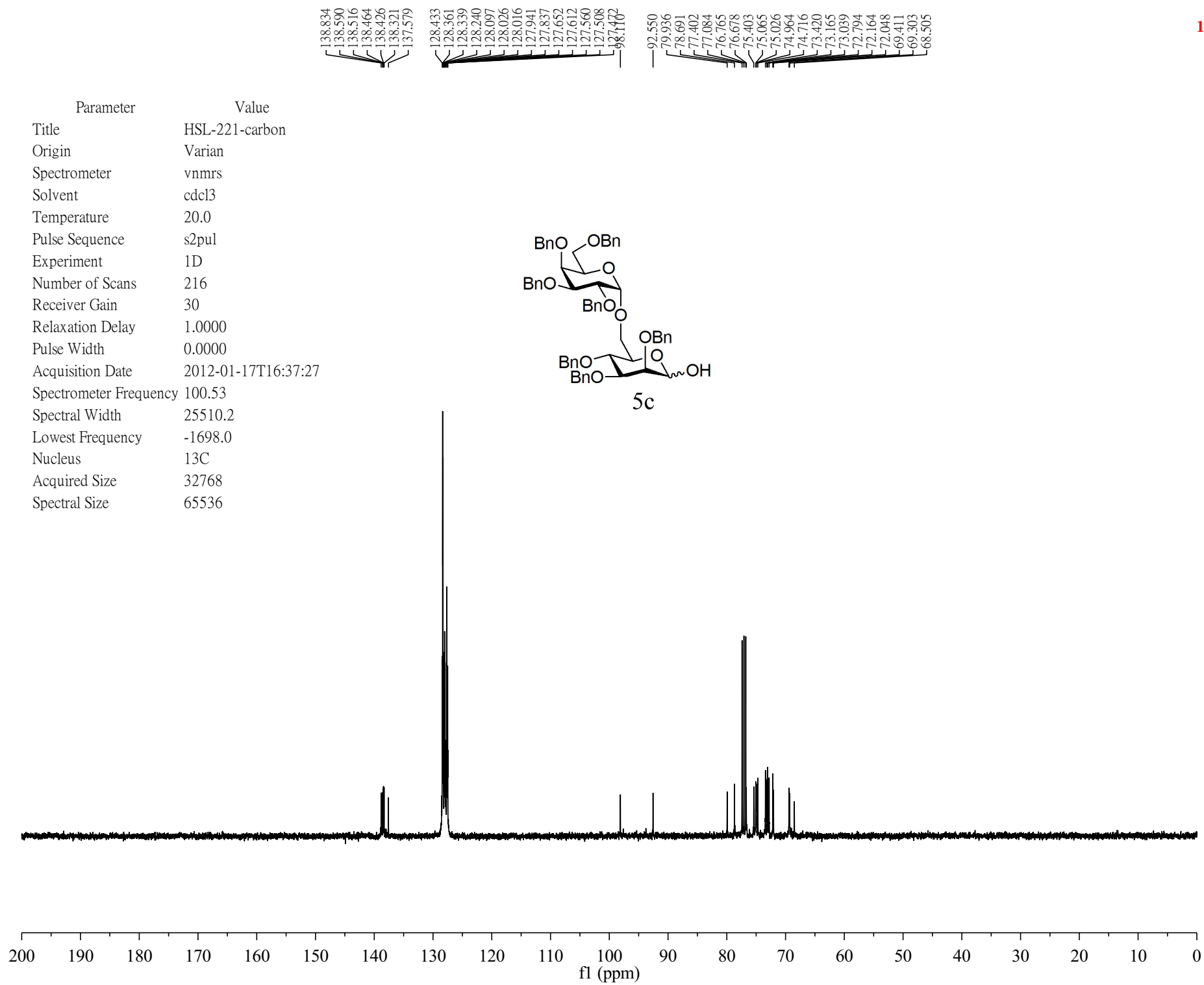


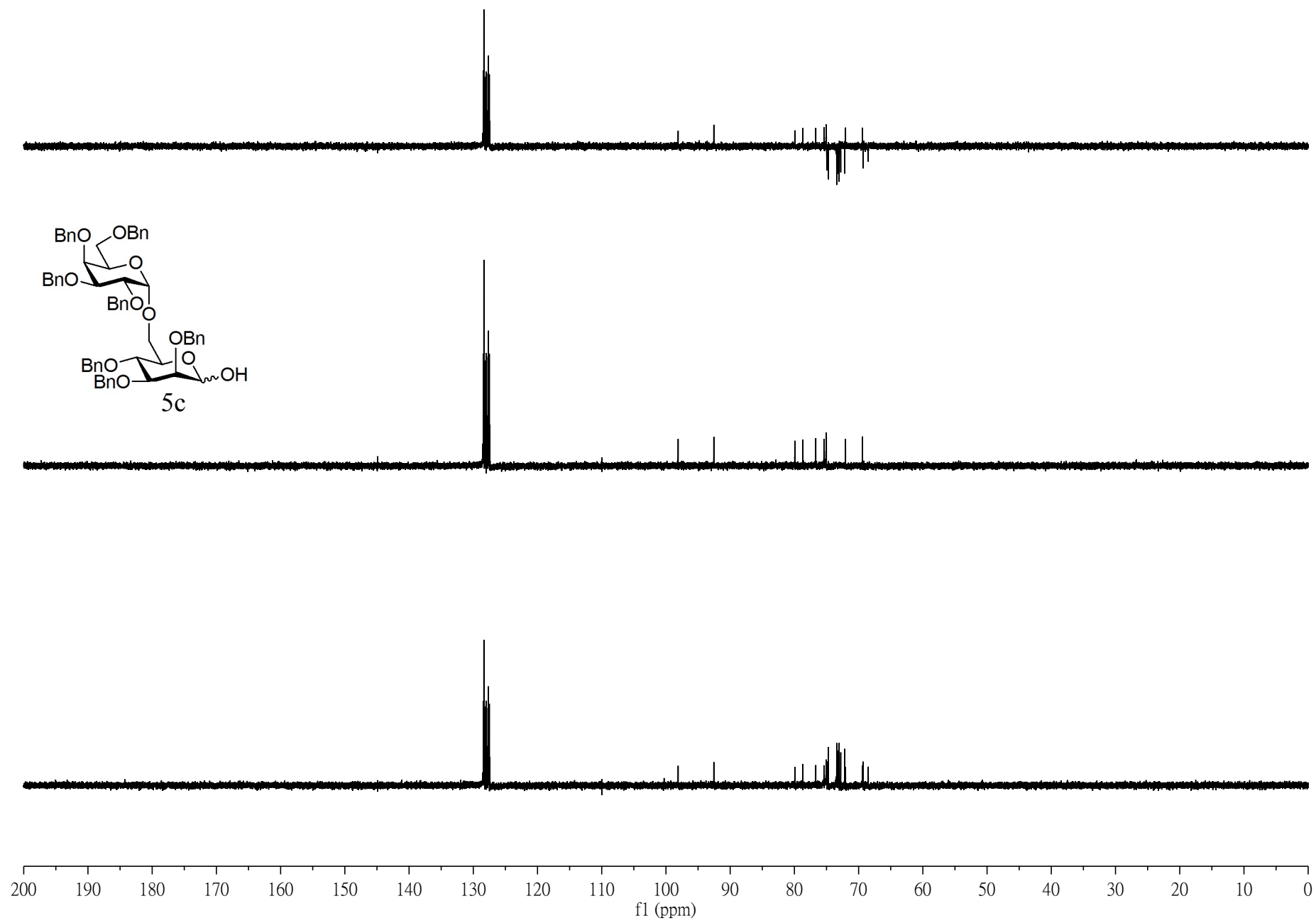
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Pulse Width	0.0000
Acquisition Date	2012-01-17T16:19:46
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Nucleus	1H
Acquired Size	16384
Spectral Size	32768

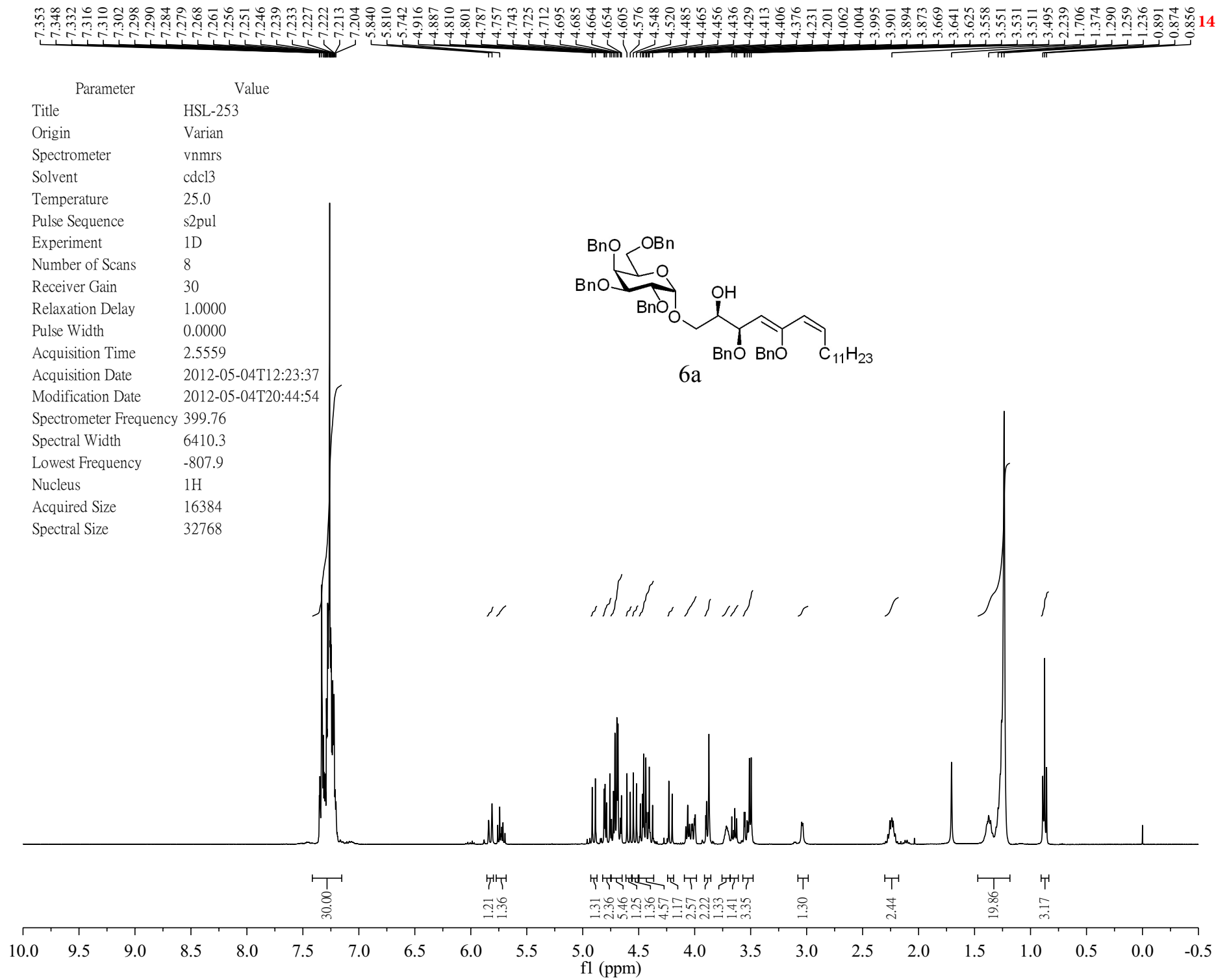


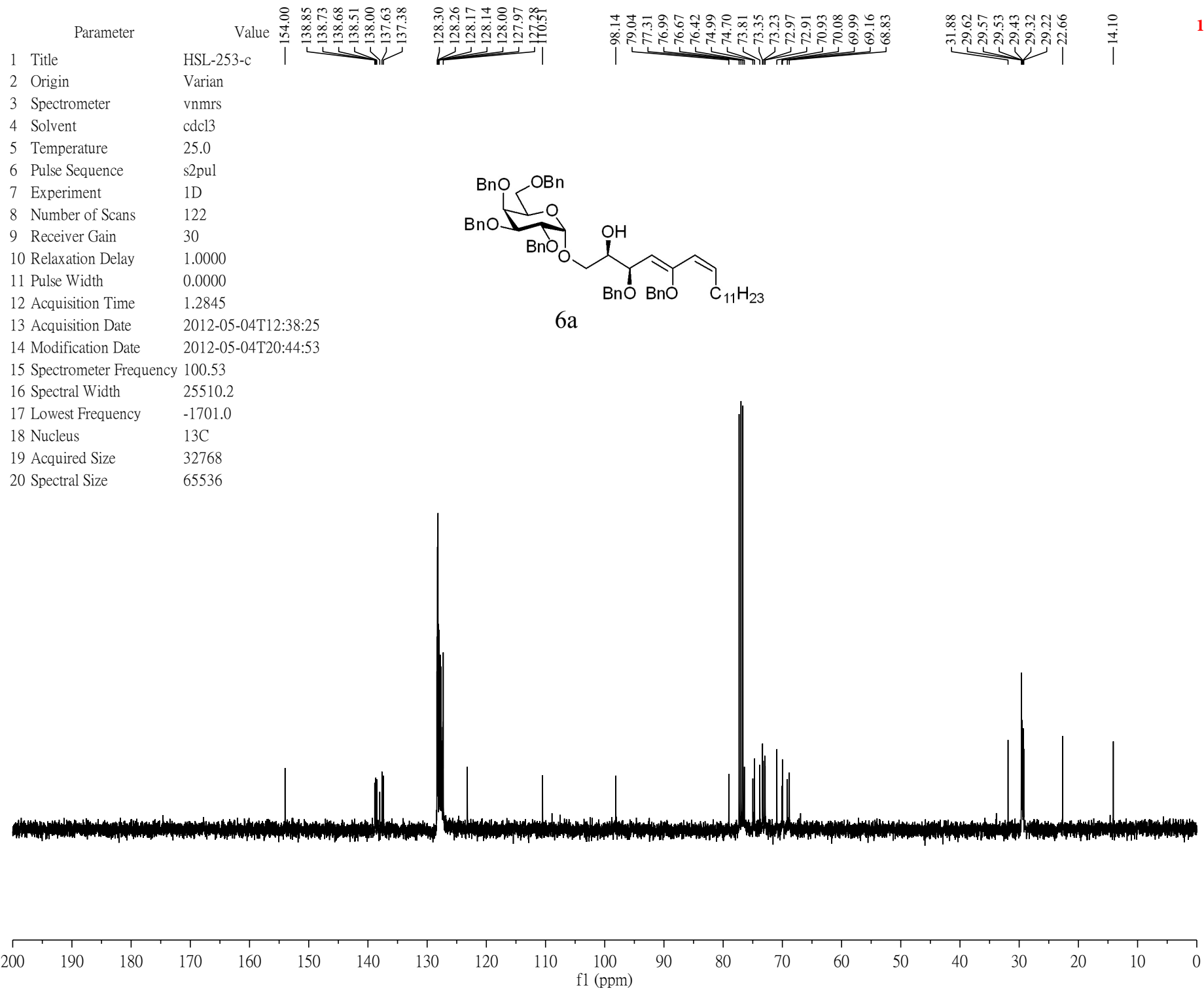
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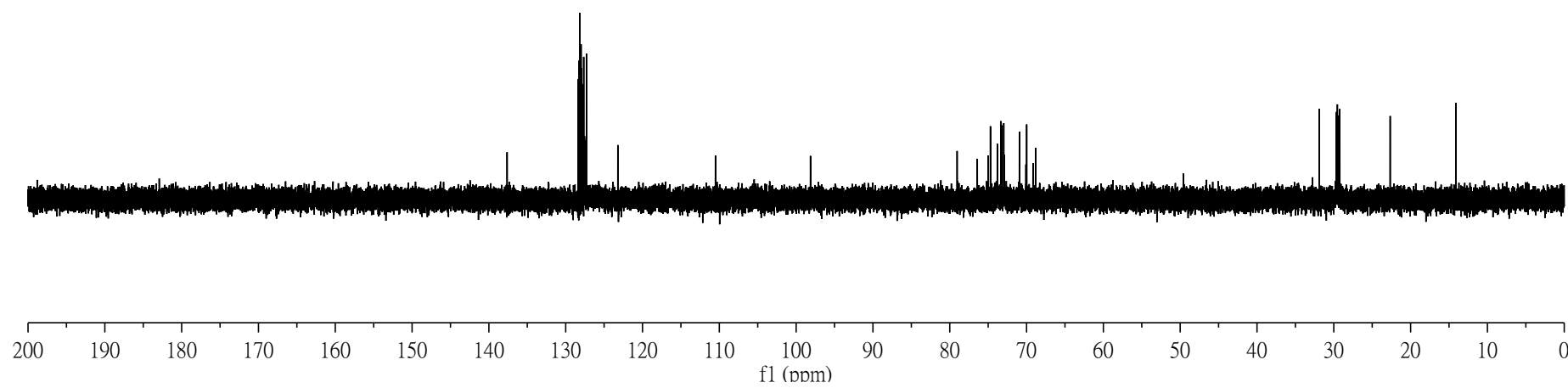
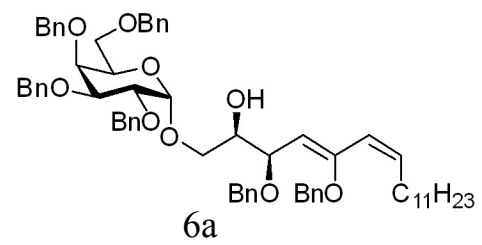
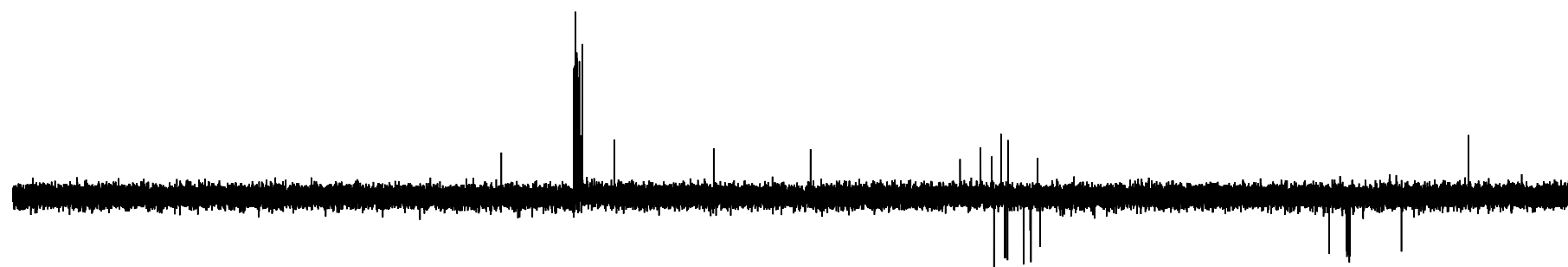
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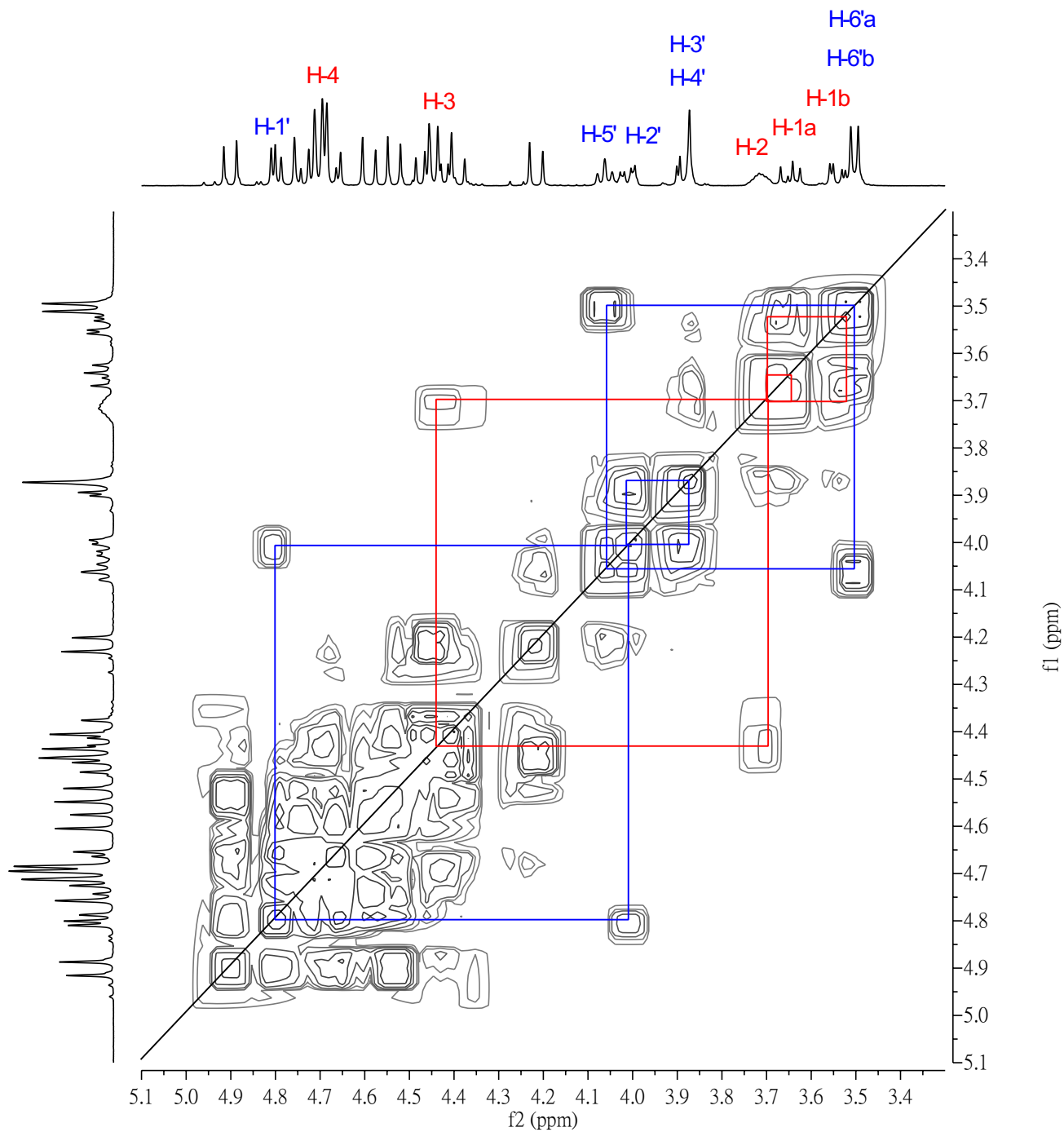
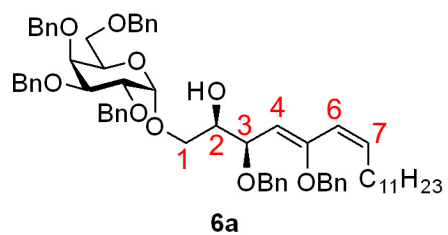




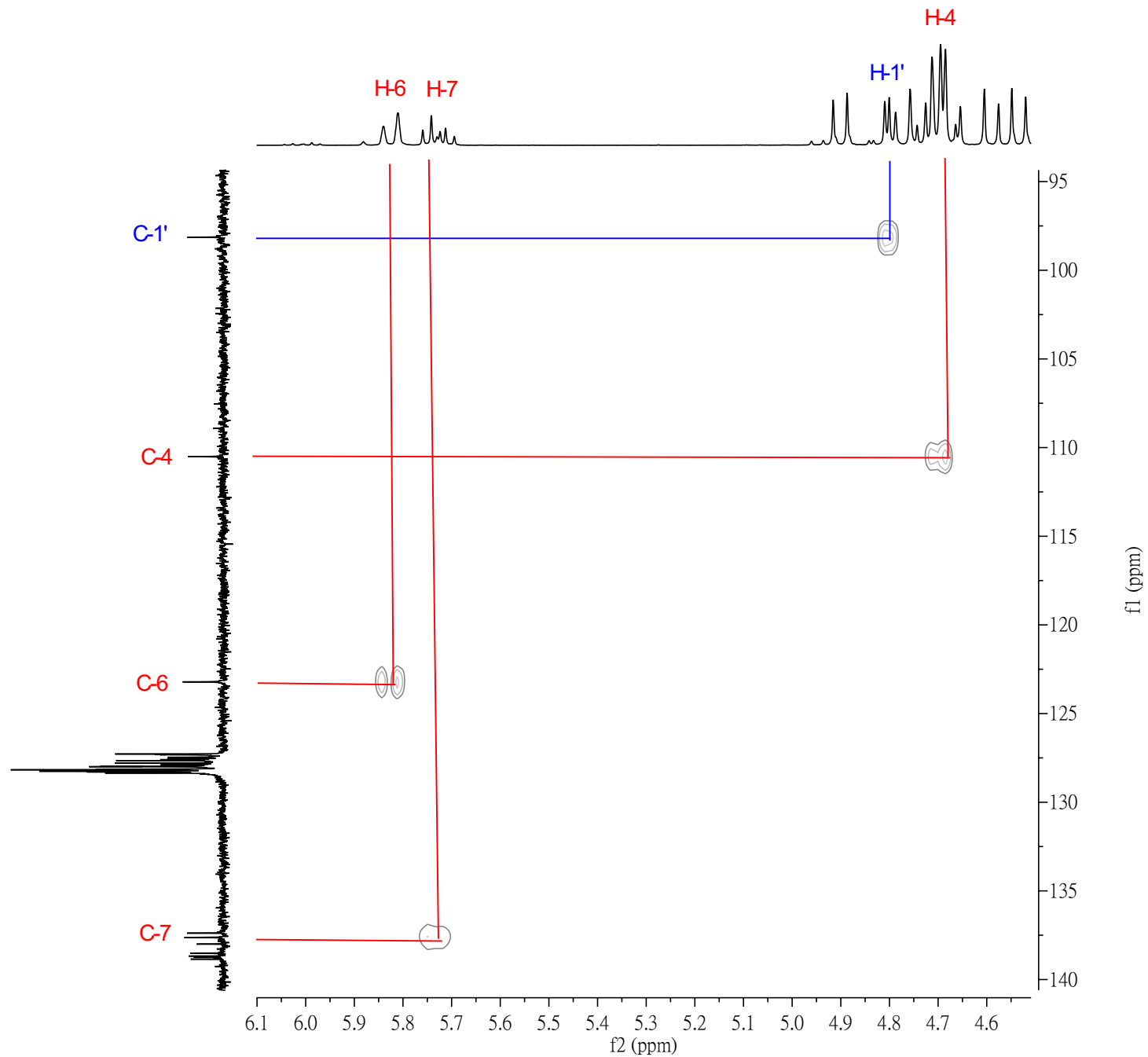
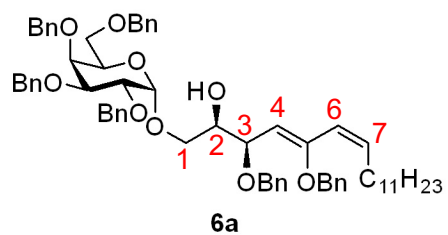




Parameter	Value (f2, f1)
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Spectrometer	nmrs
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	gCOSY
Experiment	2D-COSY
Number of Scans	1
Receiver Gain	30
Relaxation Delay	1.0000
Acquisition Time	0.1501
Spectrometer Frequency	(399.76, 399.76)
Spectral Width	(6410.3, 6410.3)
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Nucleus	(1H, 1H)
Acquired Size	(962, 128)
Spectral Size	(1024, 1024)

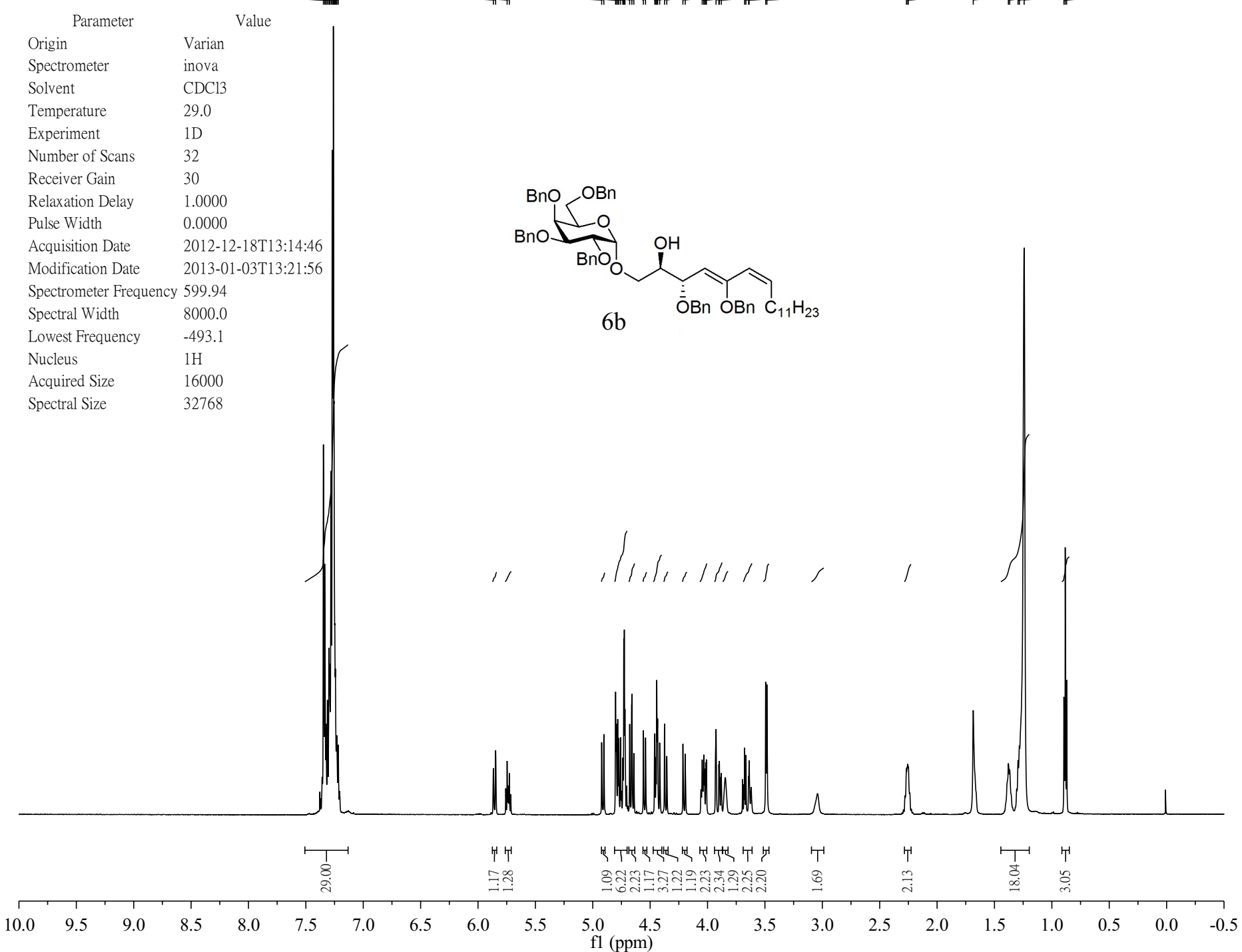
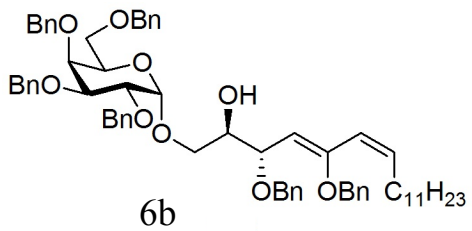


Parameter	Value (f2, f1)
Origin	Varian
Spectrometer	nmrs
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	gHSQC
Experiment	2D-HSQC-EDITED
Number of Scans	4
Receiver Gain	30
Relaxation Delay	1.0000
Acquisition Time	0.1501
Spectrometer Frequency	(399.76, 100.53)
Spectral Width	(6410.3, 17086.7)
Lowest Frequency	(-806.6, -1004.5)
Nucleus	(1H, 13C)
Acquired Size	(962, 128)
Spectral Size	(1024, 1024)



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7.323  
7.312  
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7.293  
7.291  
7.279  
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7.260  
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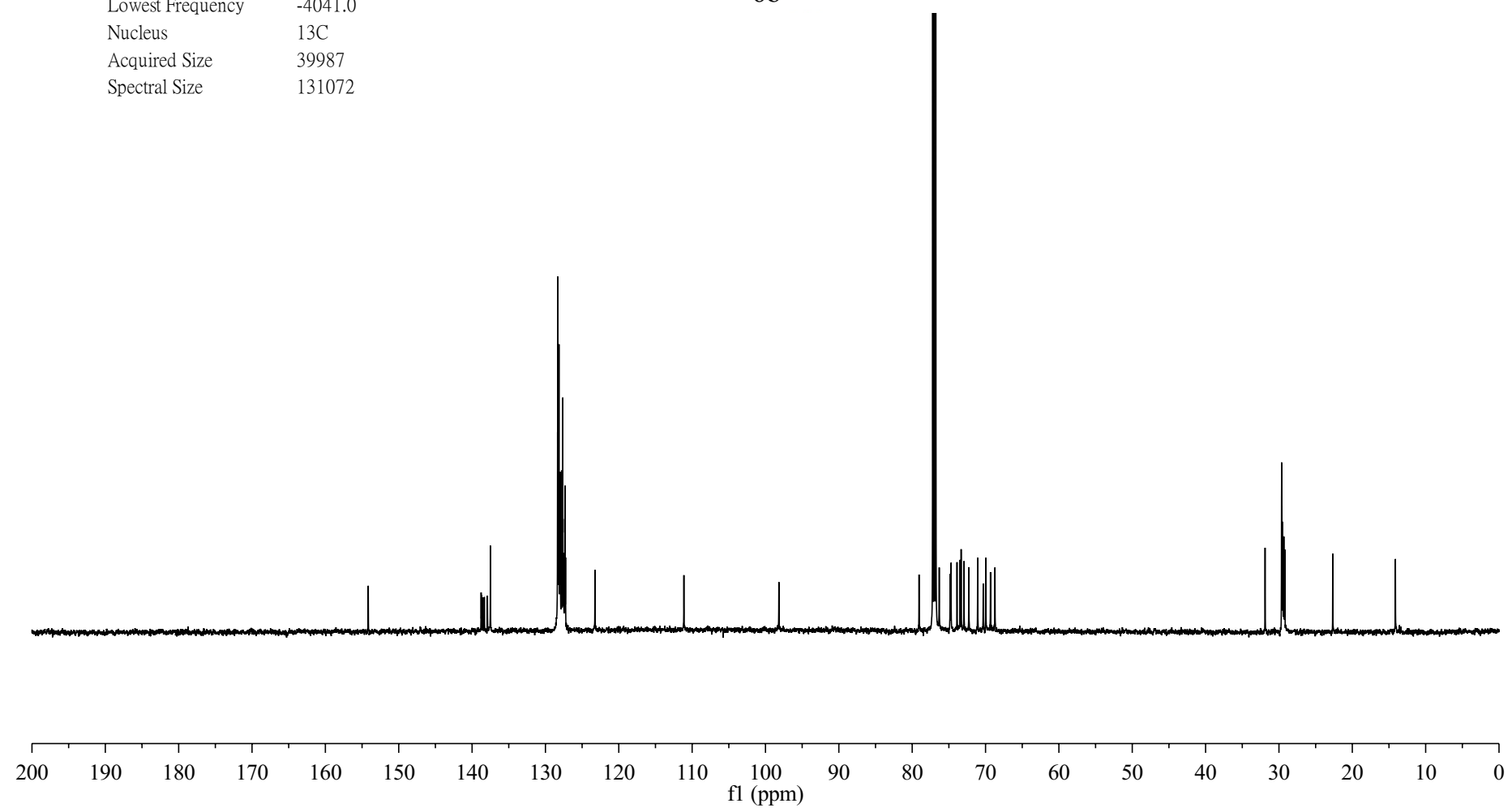
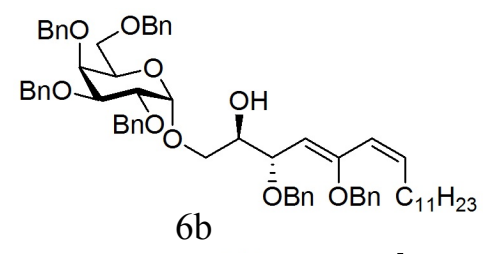
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Origin	Varian
Spectrometer	inova
Solvent	CDC13
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Experiment	1D
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Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Date	2012-12-18T13:14:46
Modification Date	2013-01-03T13:21:56
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Lowest Frequency	-493.1
Nucleus	1H
Acquired Size	16000
Spectral Size	32768

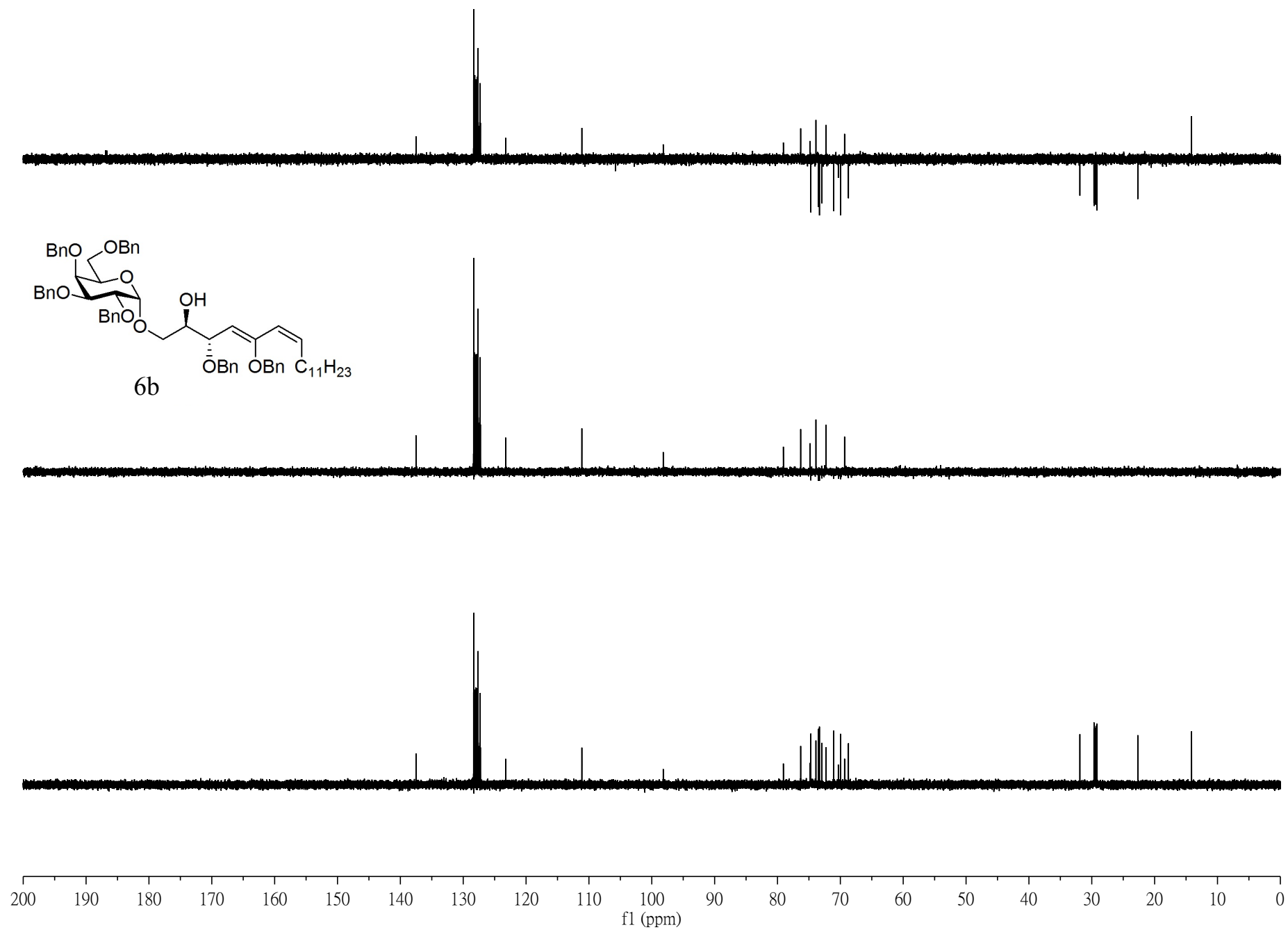


10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5  
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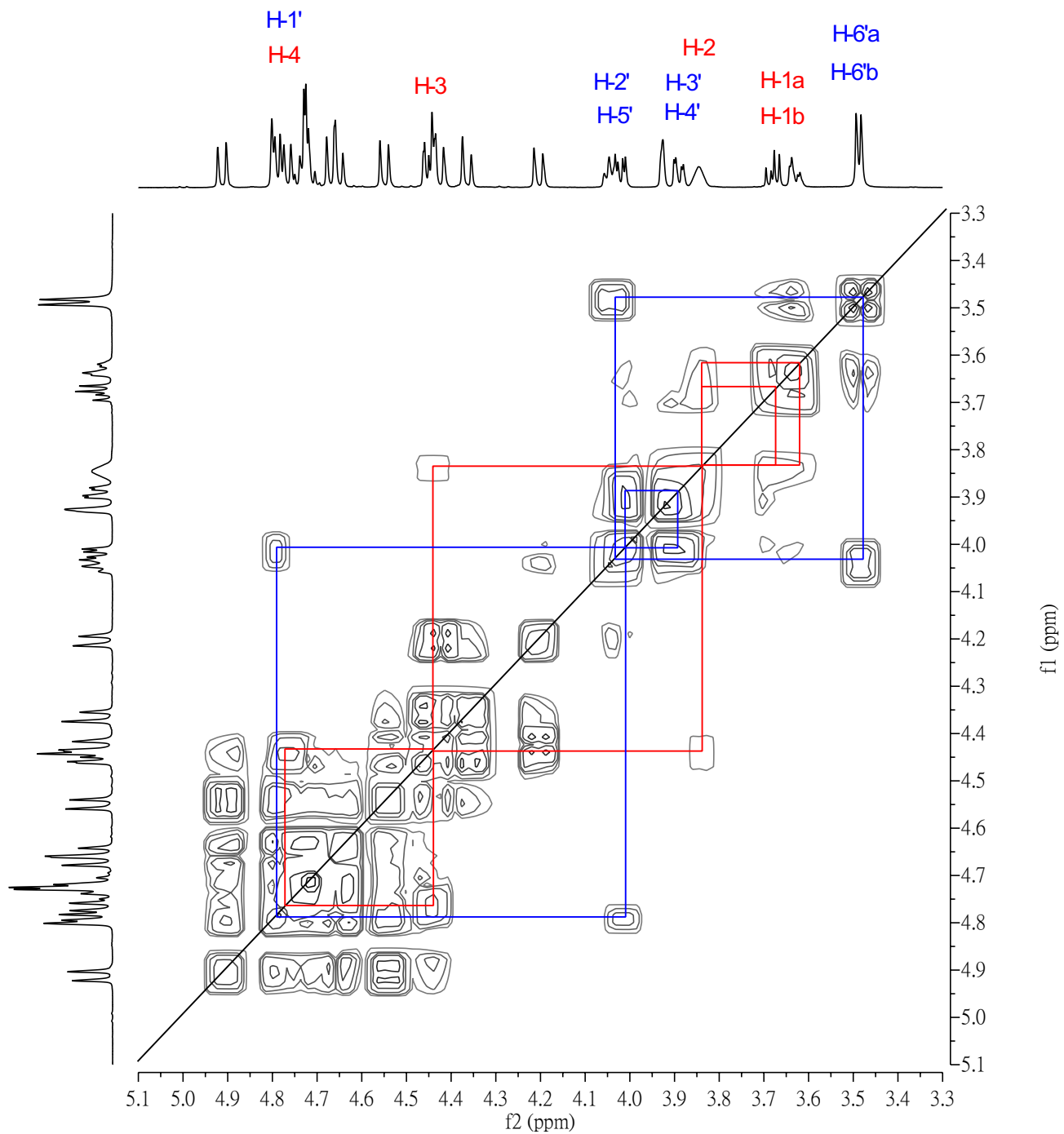
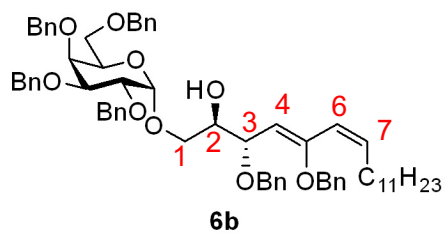
Parameter	Value
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Spectrometer	inova
Solvent	CDC13
Temperature	22.0
Experiment	1D
Number of Scans	480
Receiver Gain	58
Relaxation Delay	0.5000
Pulse Width	0.0000
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Spectrometer Frequency	150.87
Spectral Width	40000.0
Lowest Frequency	-4041.0
Nucleus	<sup>13</sup> C
Acquired Size	39987
Spectral Size	131072

- 151.52
- 138.766
- 138.707
- 138.566
- 138.330
- 137.904
- 137.499
- 128.344
- 128.311
- 128.192
- 128.153
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- 127.961
- 127.776
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- 69.970
- 69.330
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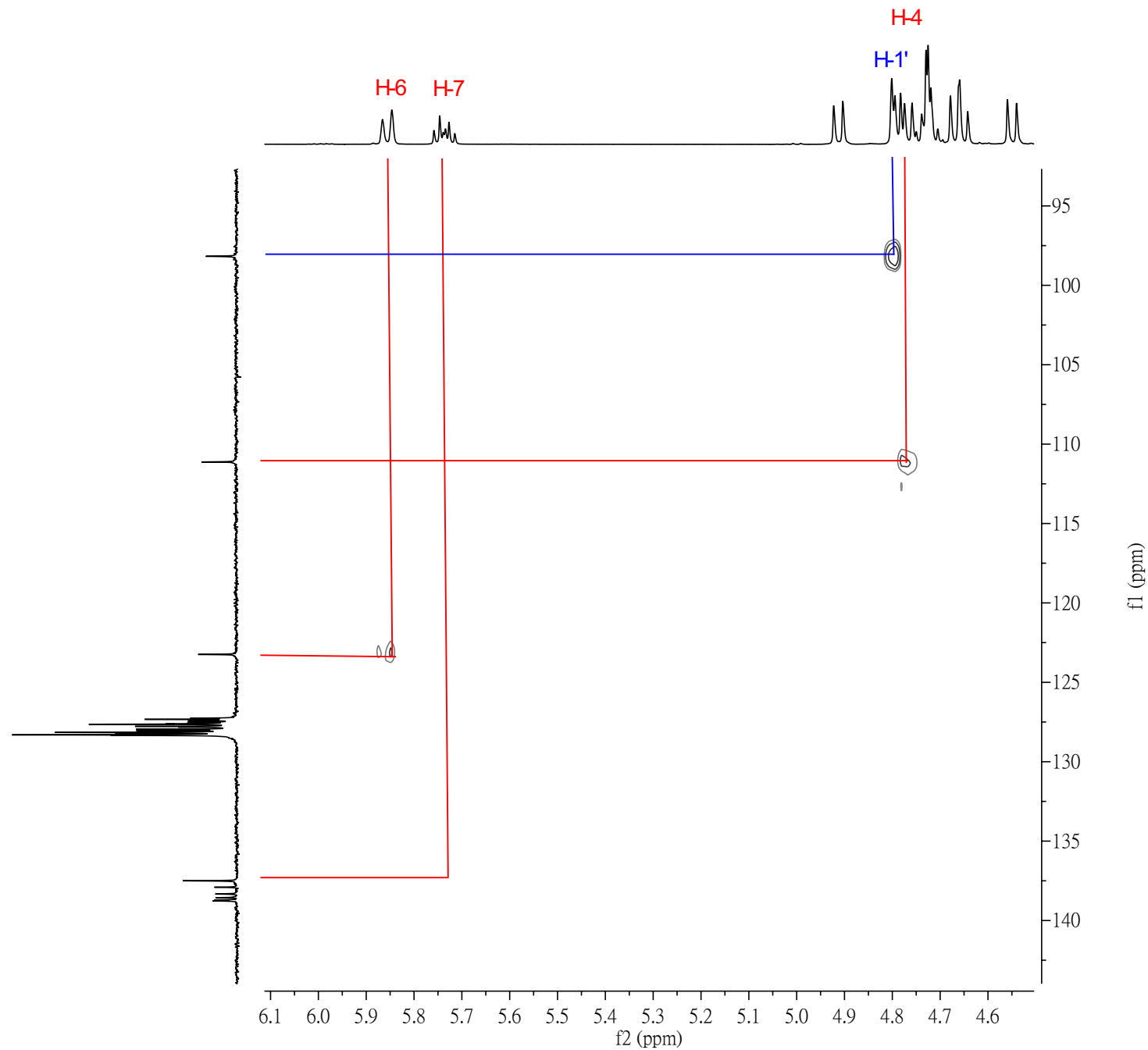
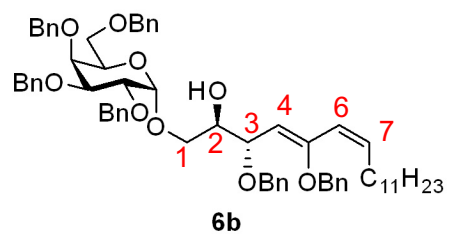


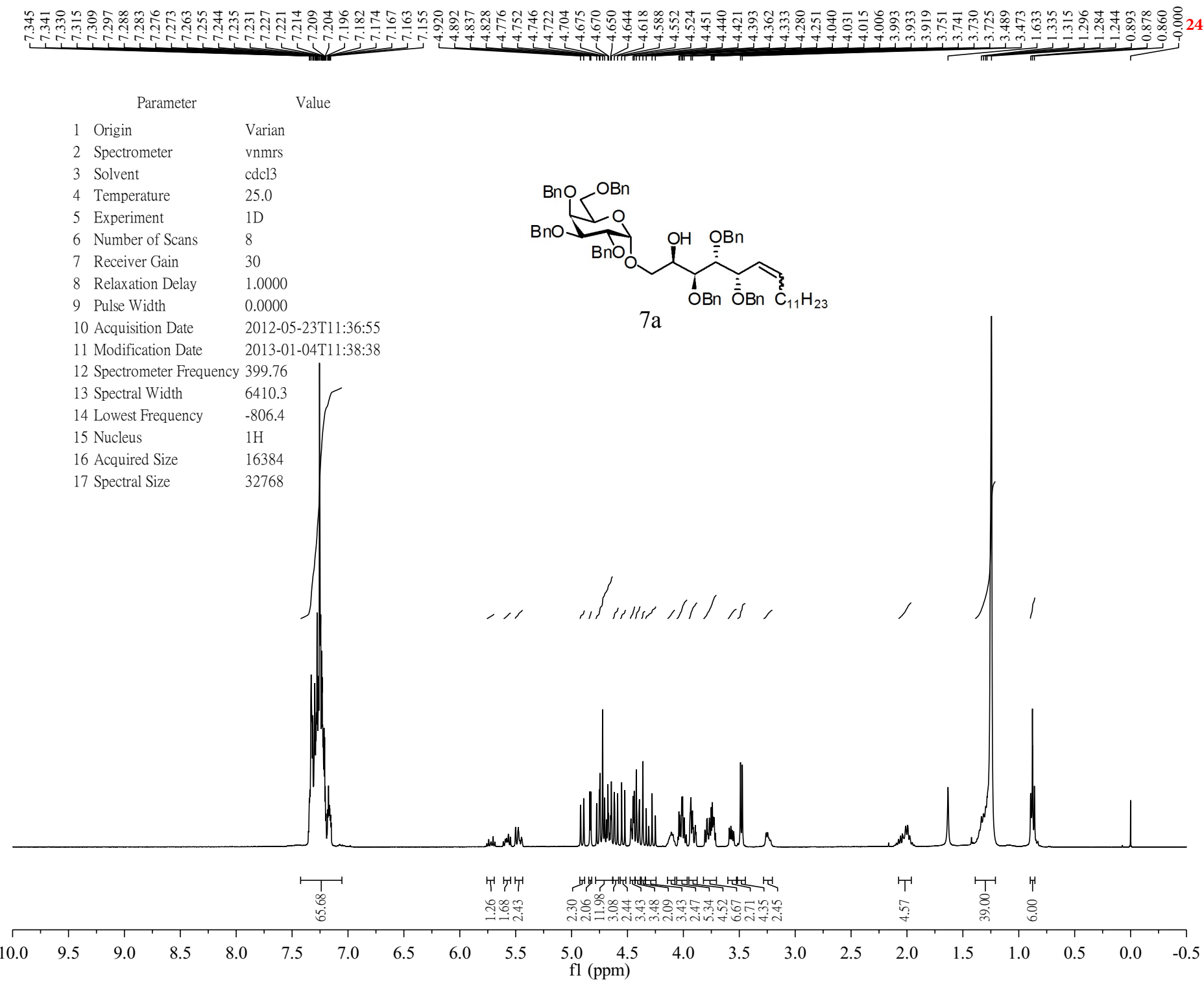


Parameter	Value (f2, f1)
Origin	Varian
Spectrometer	nmrs
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	gCOSY
Experiment	2D-COSY
Number of Scans	1
Receiver Gain	30
Relaxation Delay	1.0000
Acquisition Time	0.1501
Spectrometer Frequency	(399.76, 399.76)
Spectral Width	(6410.3, 6410.3)
Lowest Frequency	(-810.9, -810.9)
Nucleus	(1H, 1H)
Acquired Size	(962, 128)
Spectral Size	(1024, 1024)

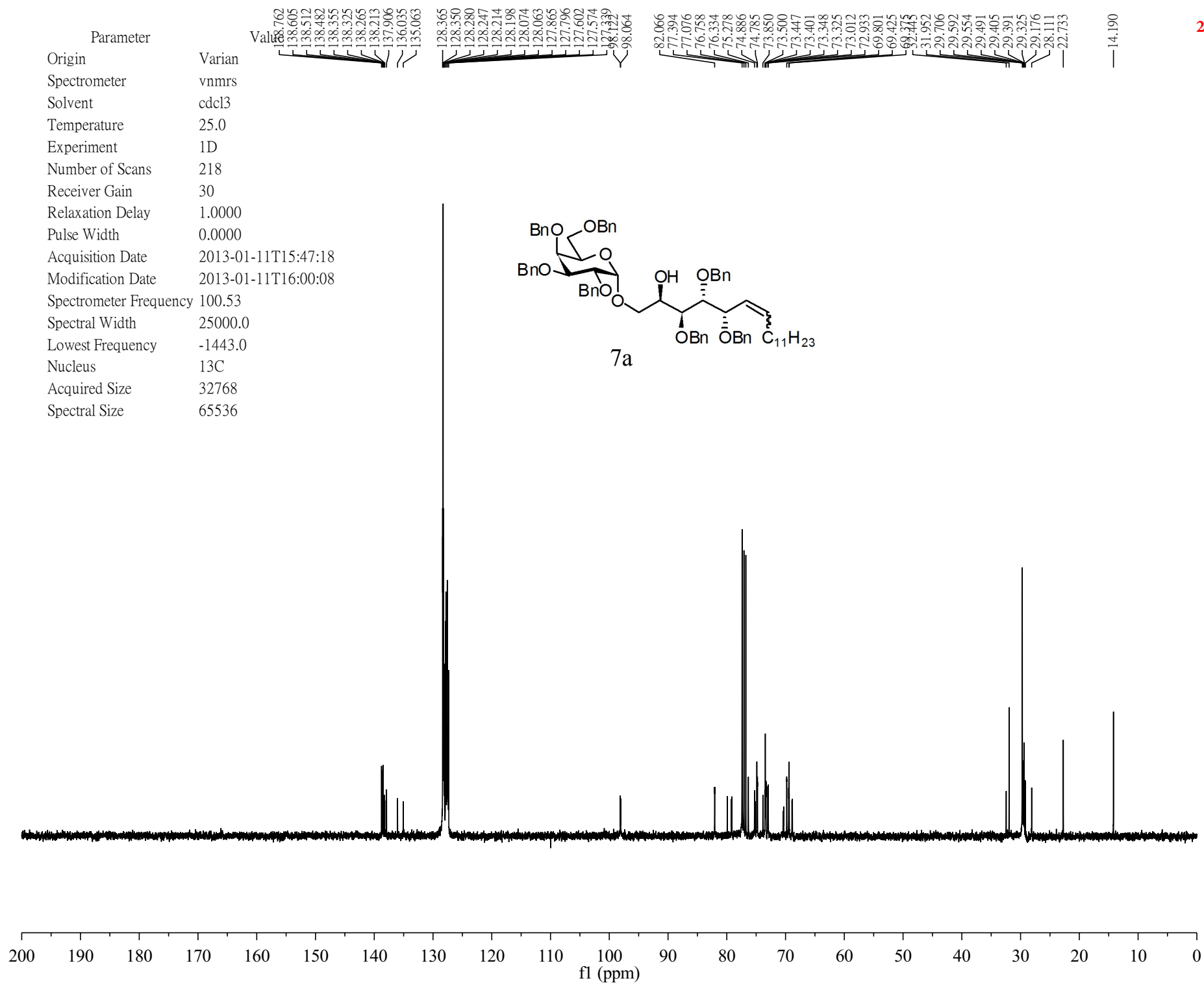


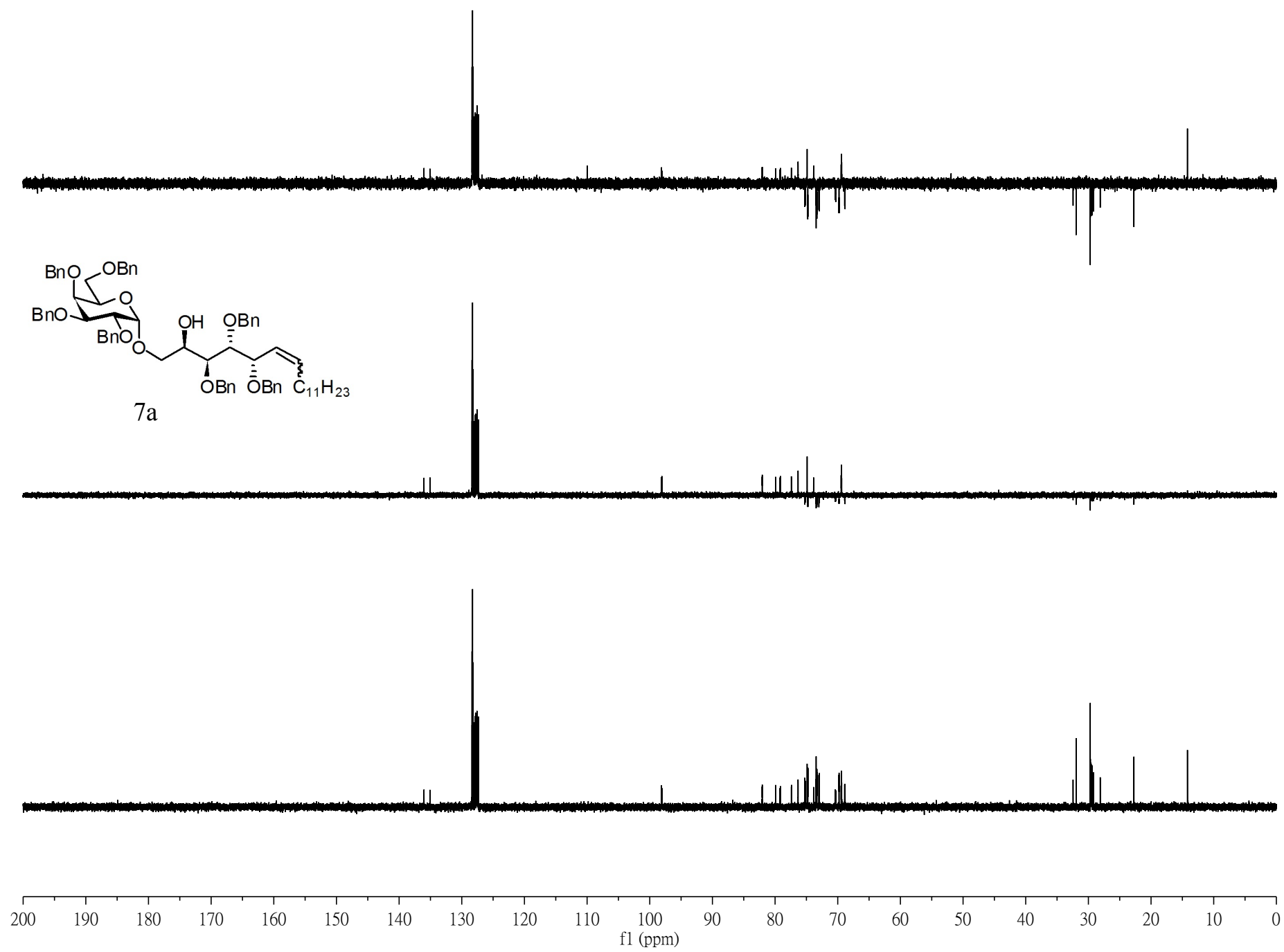
Parameter	Value (f2, f1)
Origin	Varian
Spectrometer	inova
Solvent	CDCl <sub>3</sub>
Temperature	29.0
Pulse Sequence	gHSQC
Experiment	2D-HSQC
Number of Scans	16
Receiver Gain	50
Relaxation Delay	1.0000
Acquisition Time	0.1280
Spectrometer Frequency	(599.94, 150.86)
Spectral Width	(8000.0, 25641.0)
Lowest Frequency	(-491.2, -1529.6)
Nucleus	( <sup>1</sup> H, <sup>13</sup> C)
Acquired Size	(1024, 128)
Spectral Size	(1024, 1024)

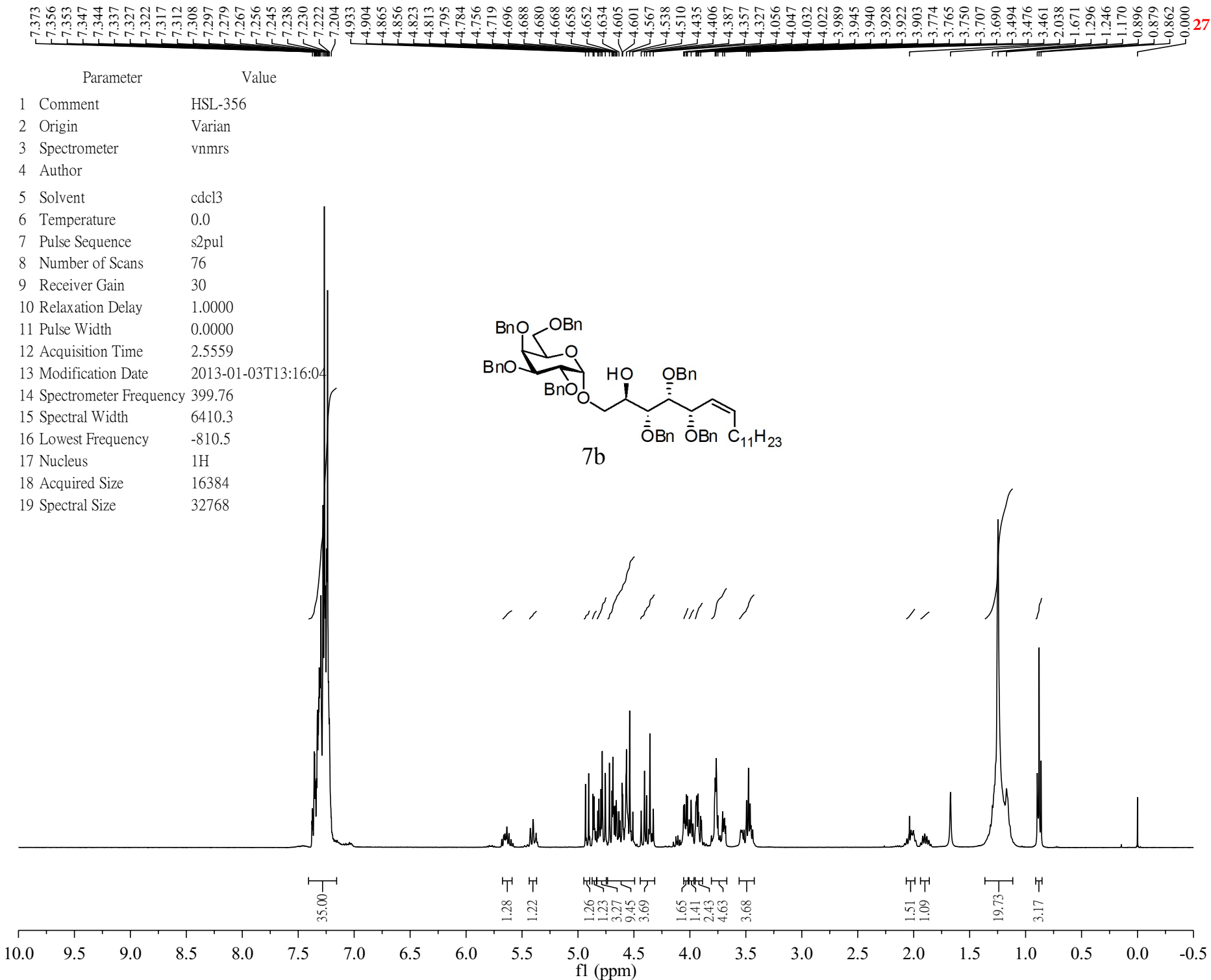










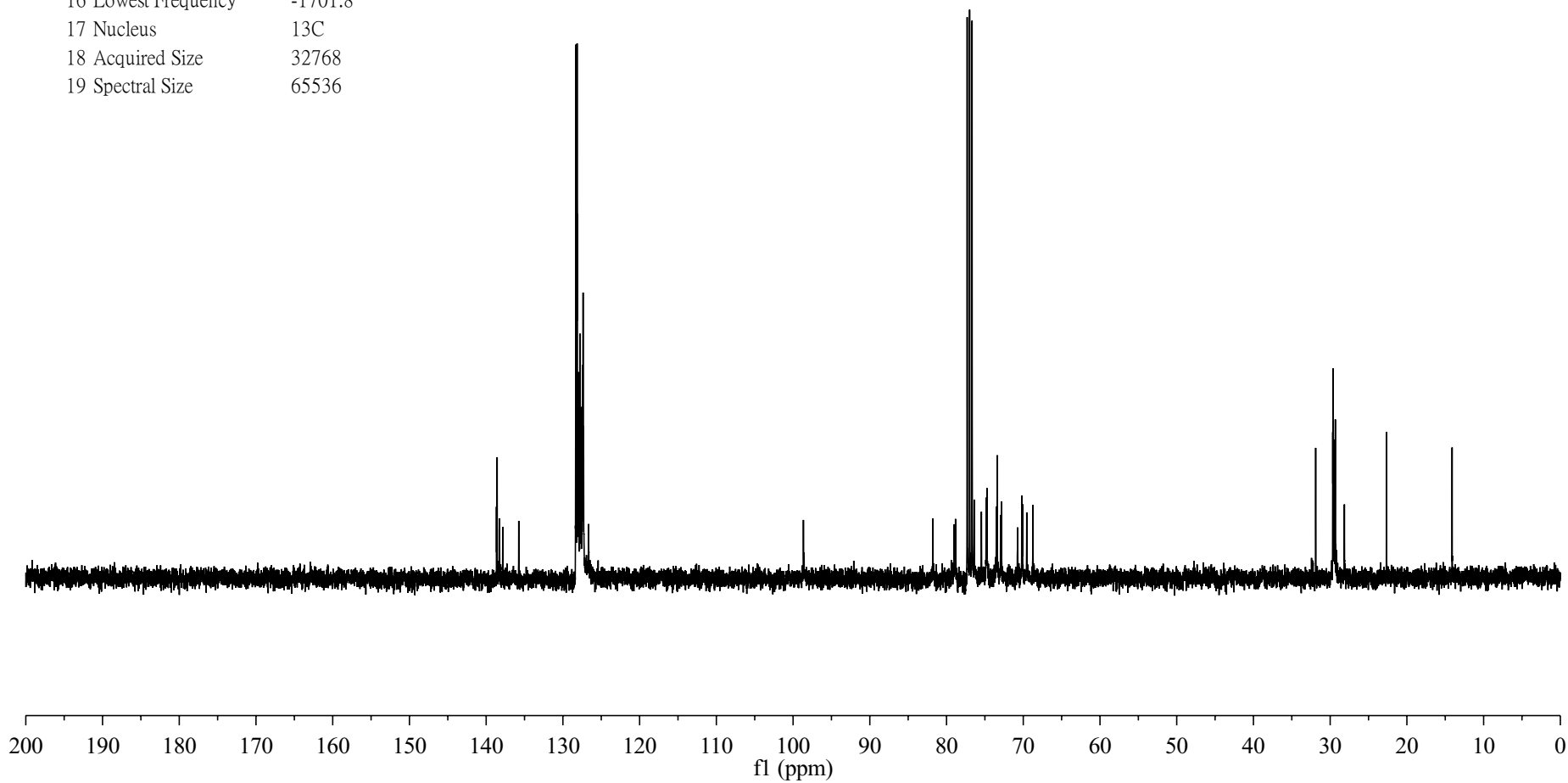
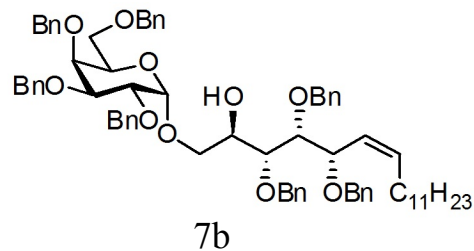


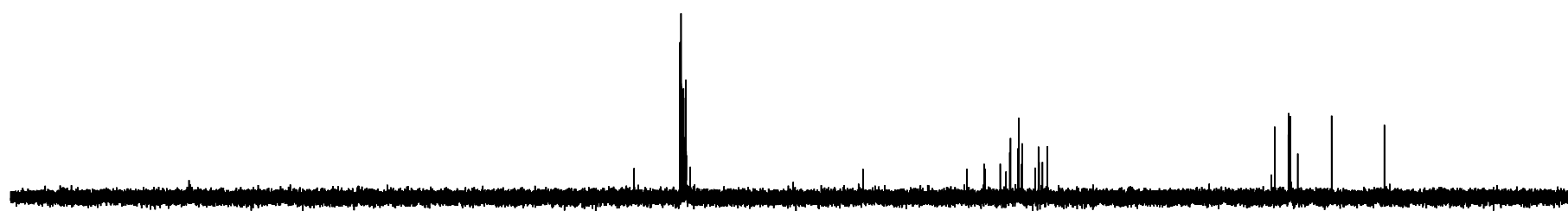
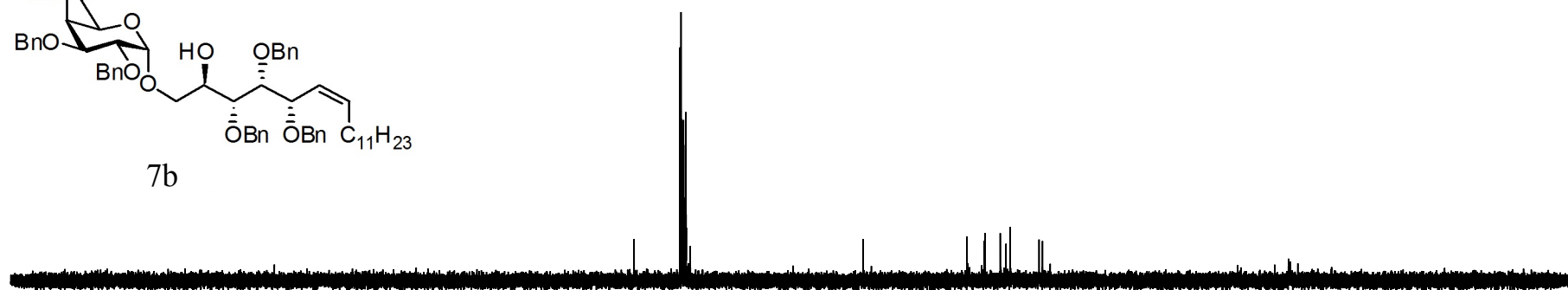
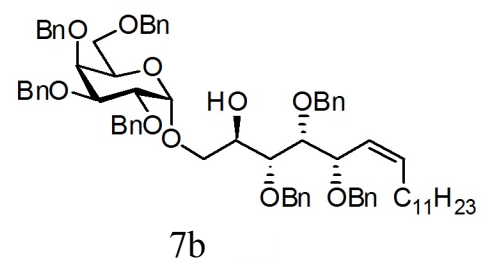
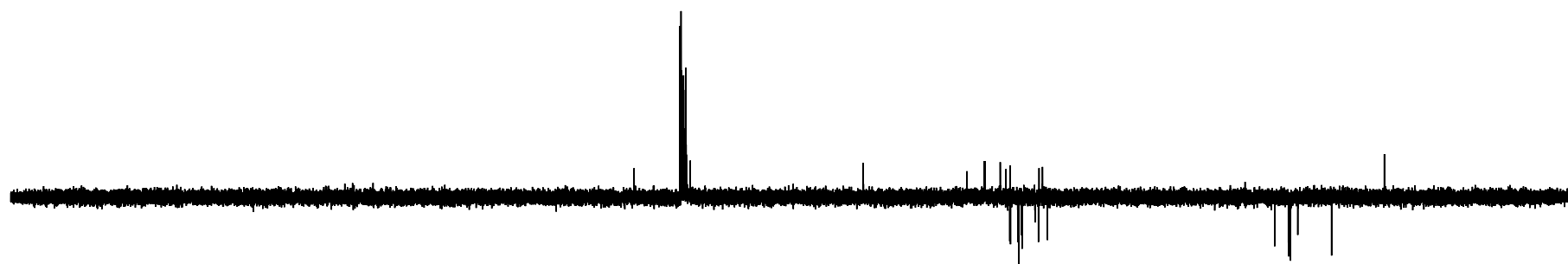
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8 Number of Scans	128
9 Receiver Gain	30
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.2845
13 Modification Date	2013-01-03T13:16:00
14 Spectrometer Frequency	100.53
15 Spectral Width	25510.2
16 Lowest Frequency	-1701.8
17 Nucleus	13C
18 Acquired Size	32768
19 Spectral Size	65536

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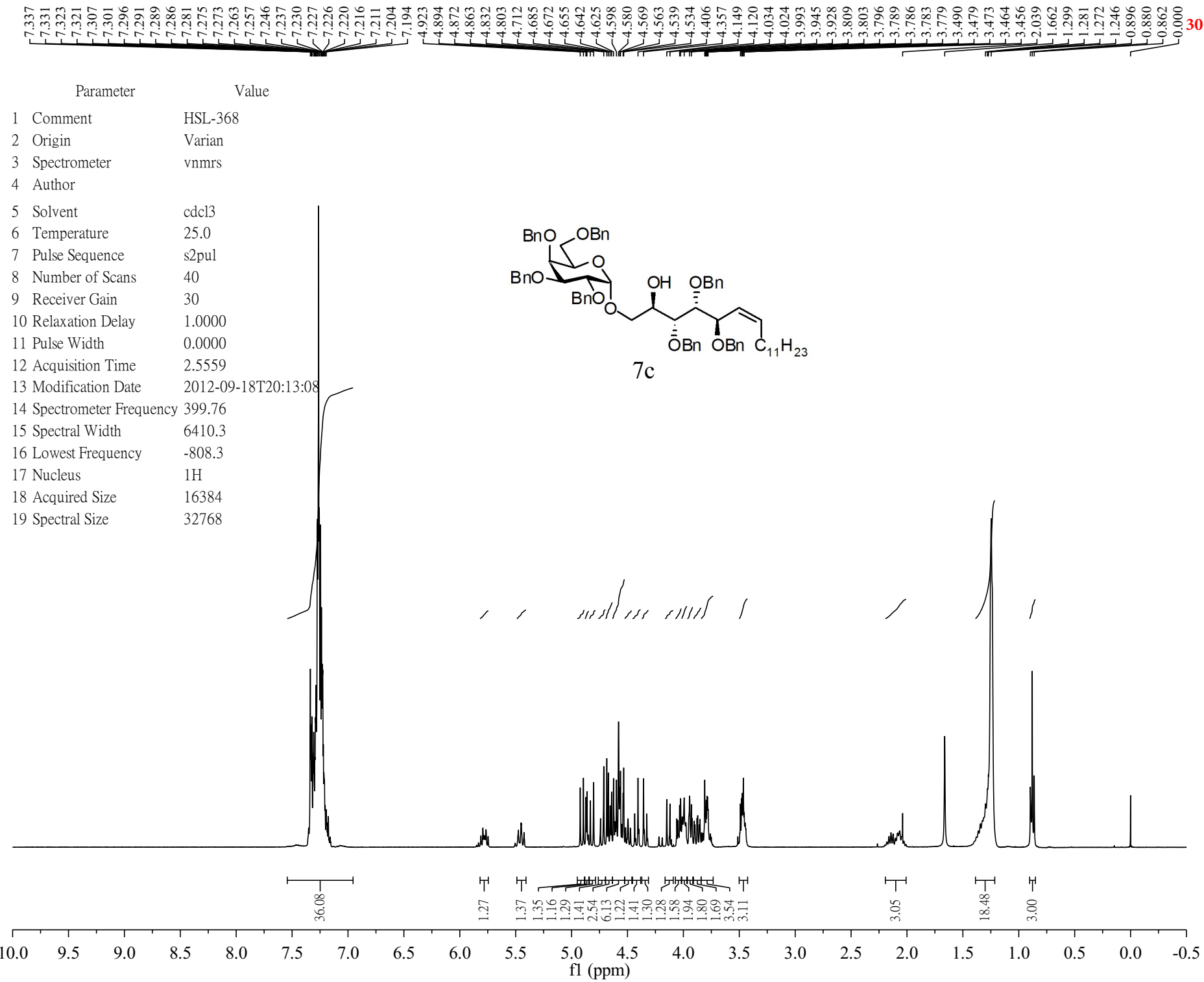
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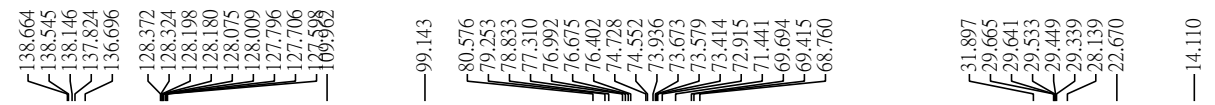
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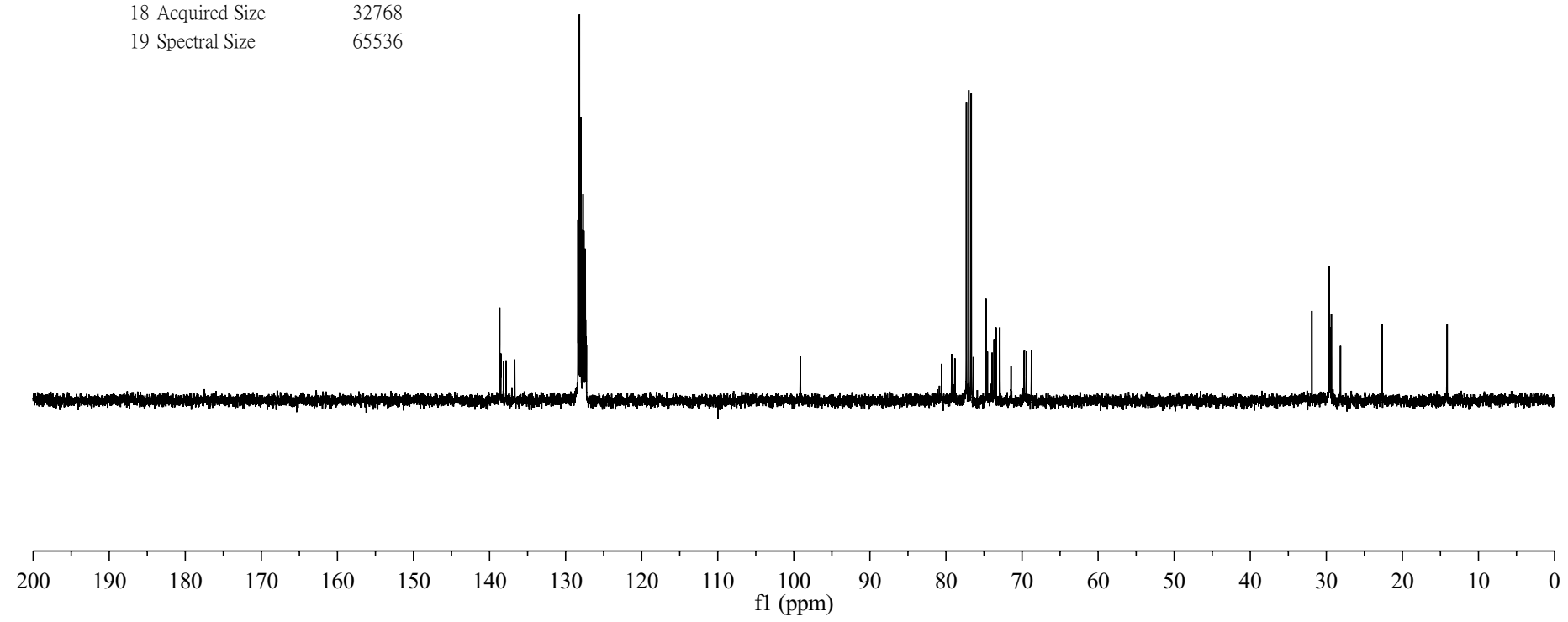
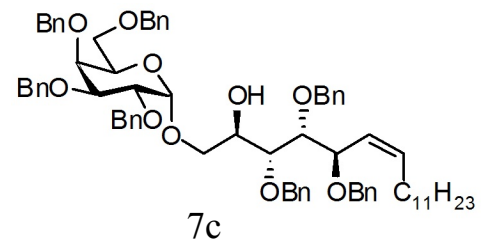


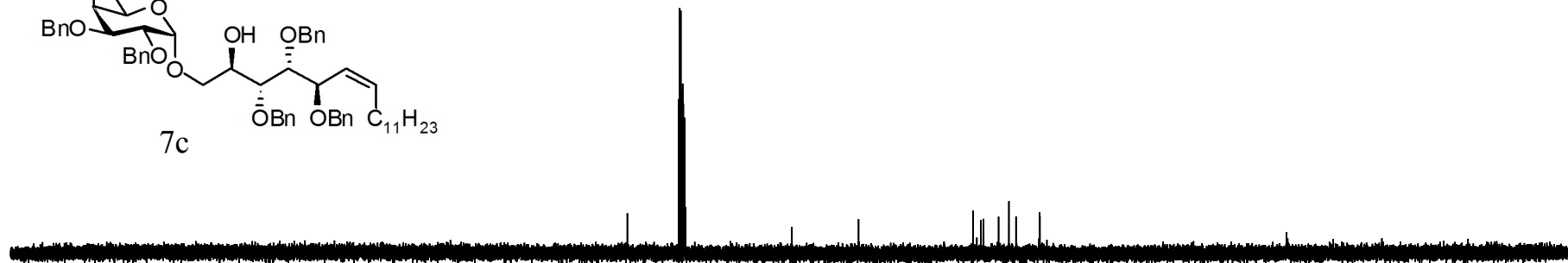
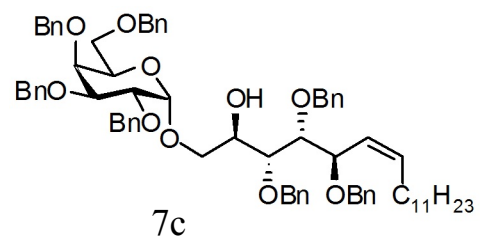
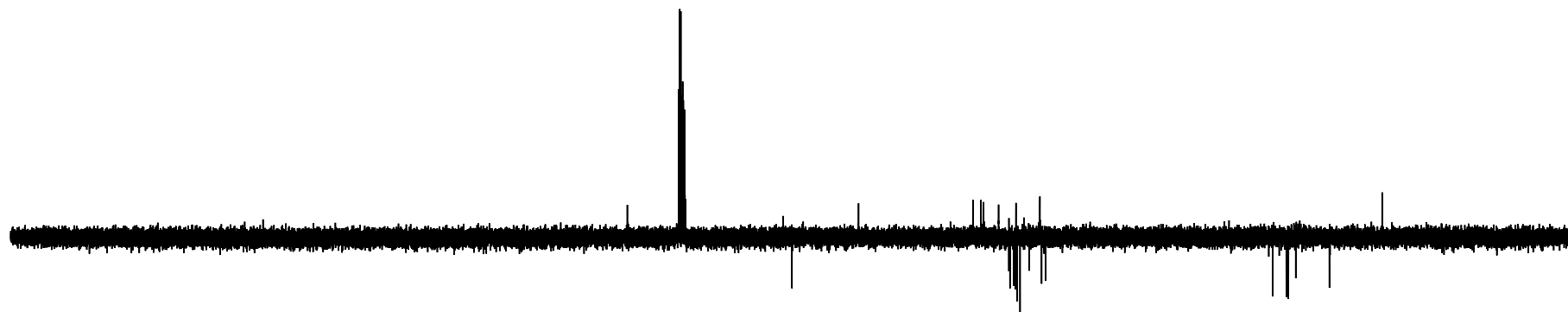
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10  
f1 (ppm)





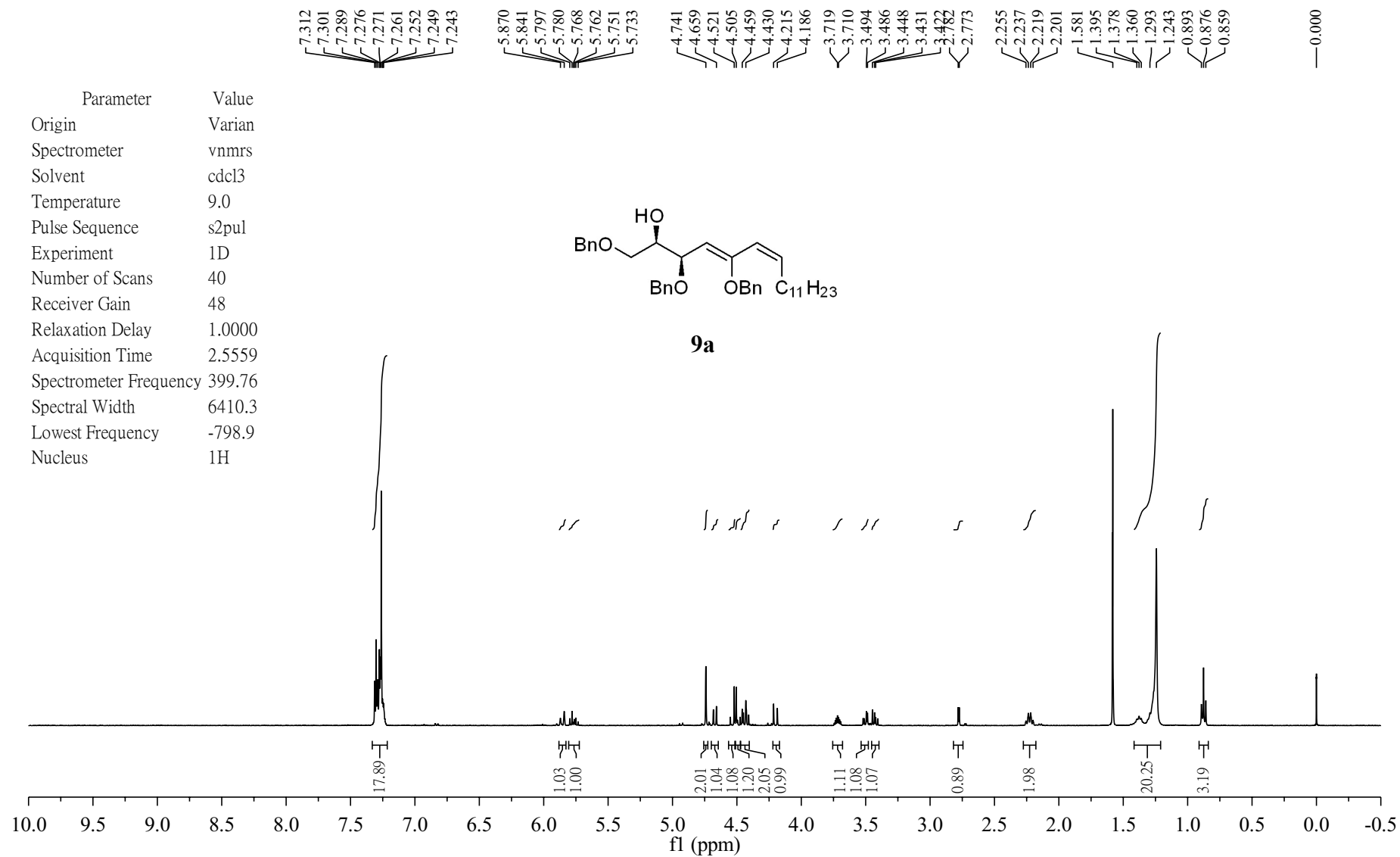
Parameter	Value
1 Comment	HSL-368
2 Origin	Varian
3 Spectrometer	vnmrs
4 Author	
5 Solvent	cdcl3
6 Temperature	25.0
7 Pulse Sequence	s2pul
8 Number of Scans	168
9 Receiver Gain	30
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.2845
13 Modification Date	2012-09-18T20:13:04
14 Spectrometer Frequency	100.53
15 Spectral Width	25510.2
16 Lowest Frequency	-1700.6
17 Nucleus	13C
18 Acquired Size	32768
19 Spectral Size	65536

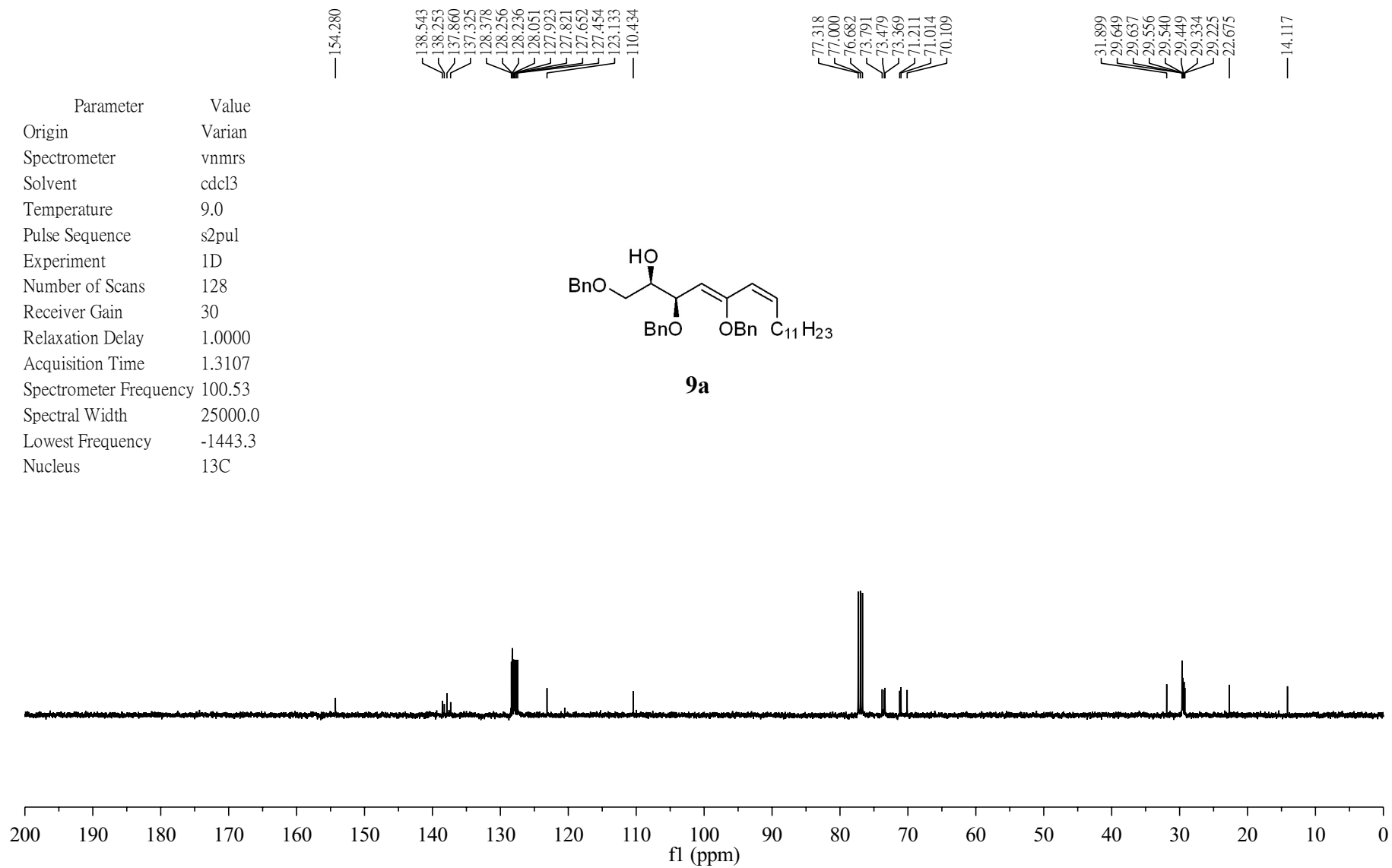


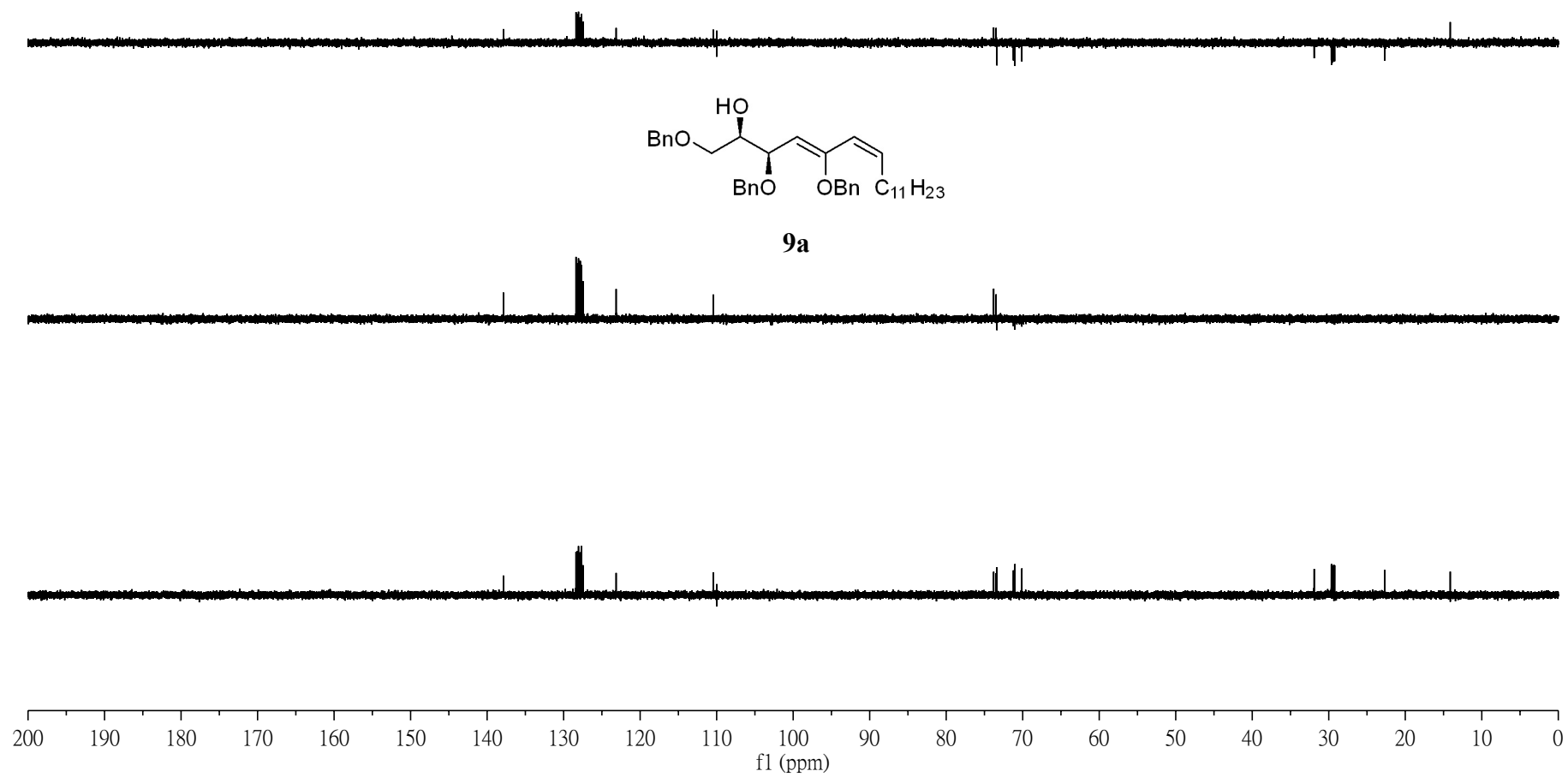


230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10  
f1 (ppm)

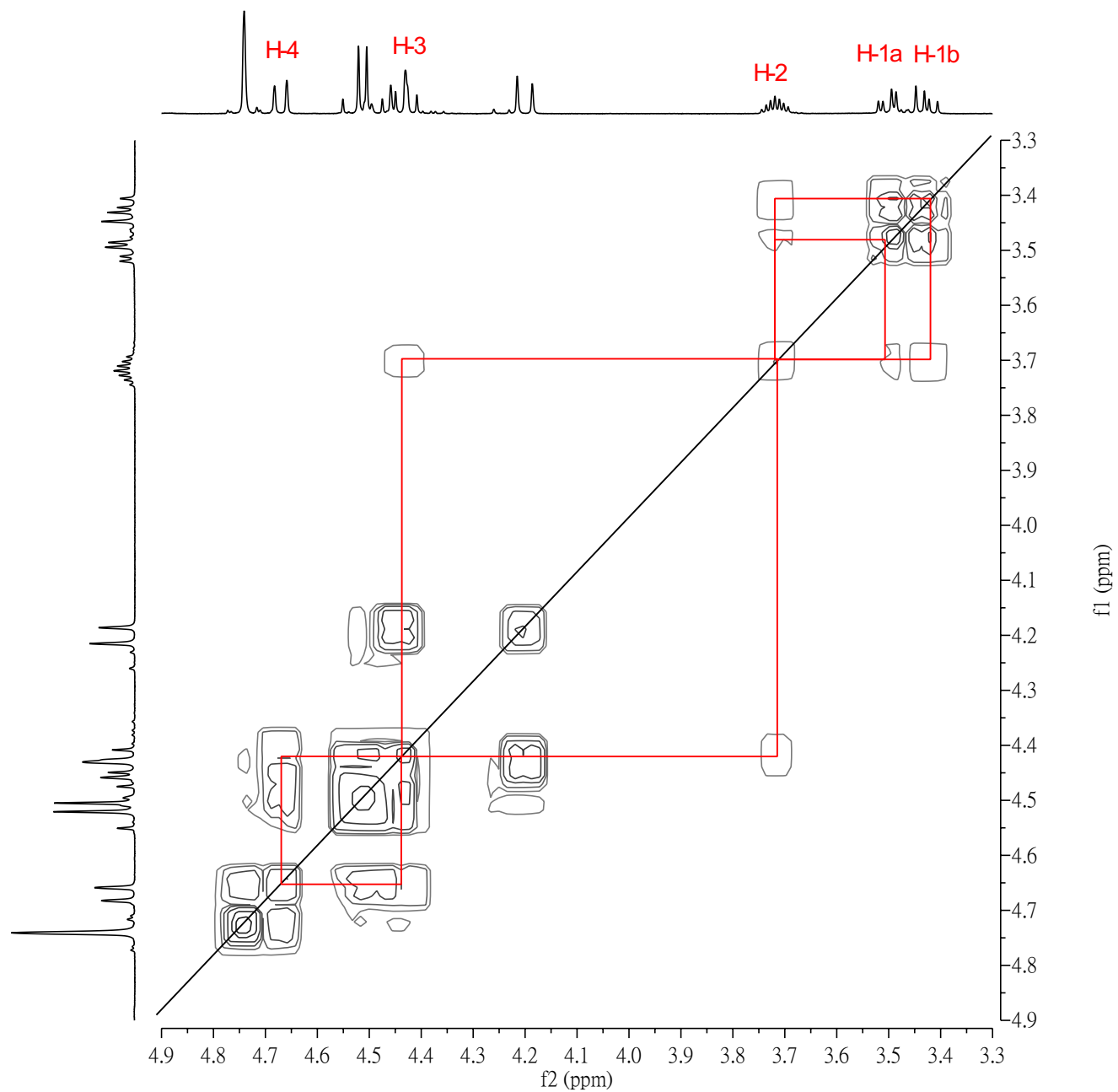
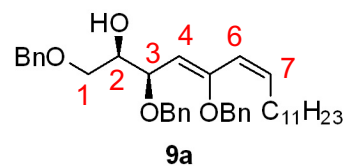




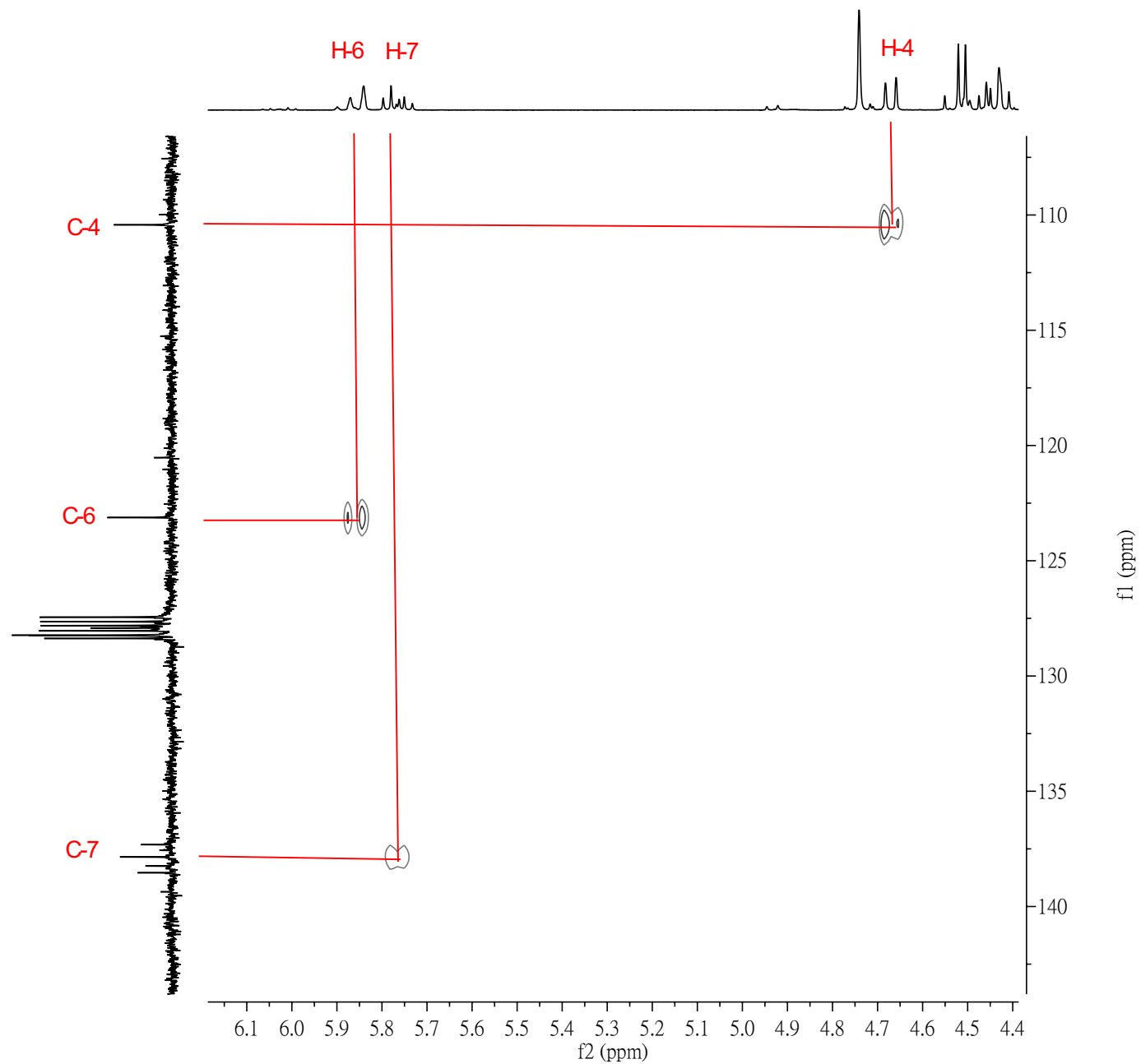
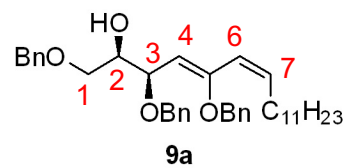


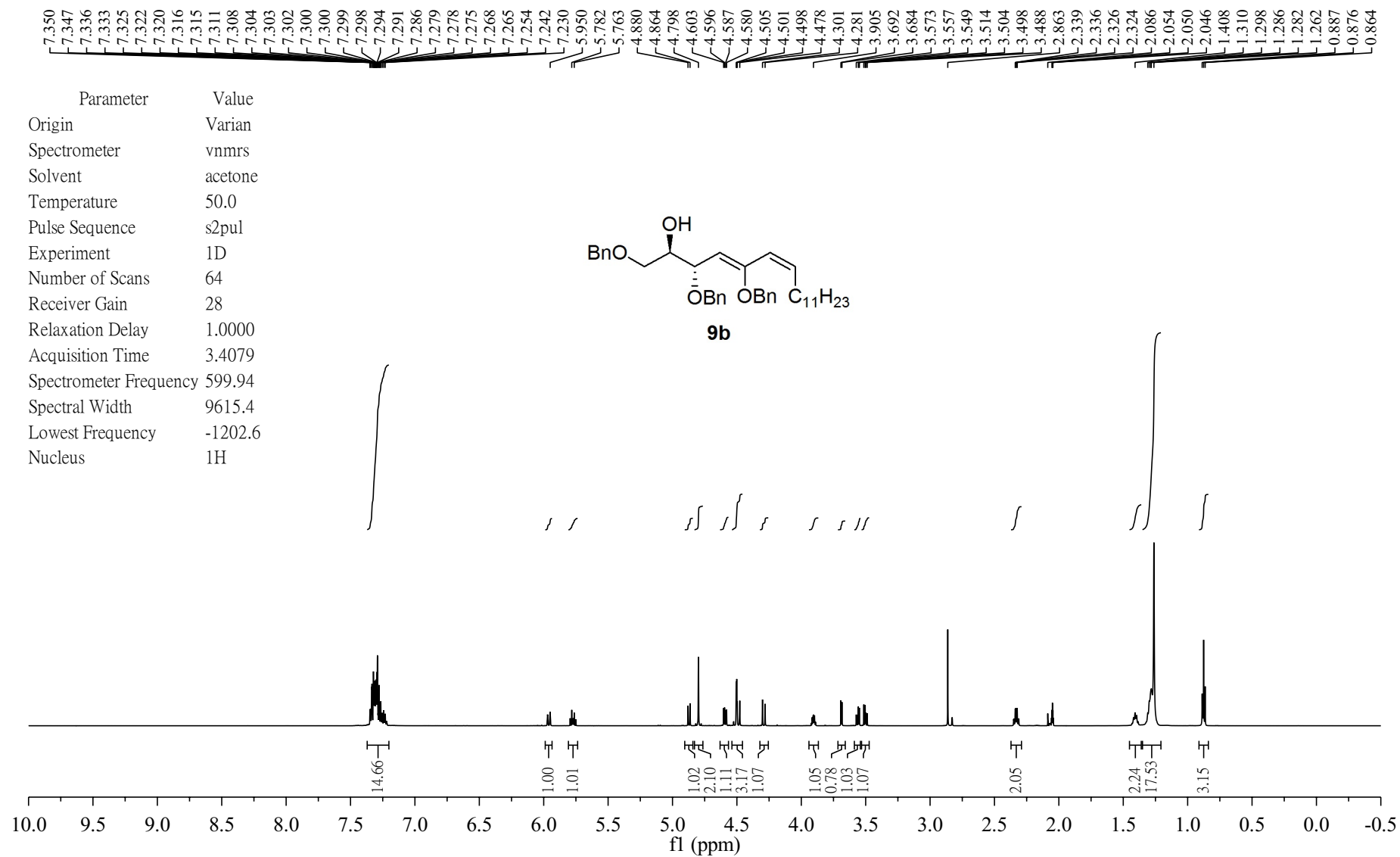


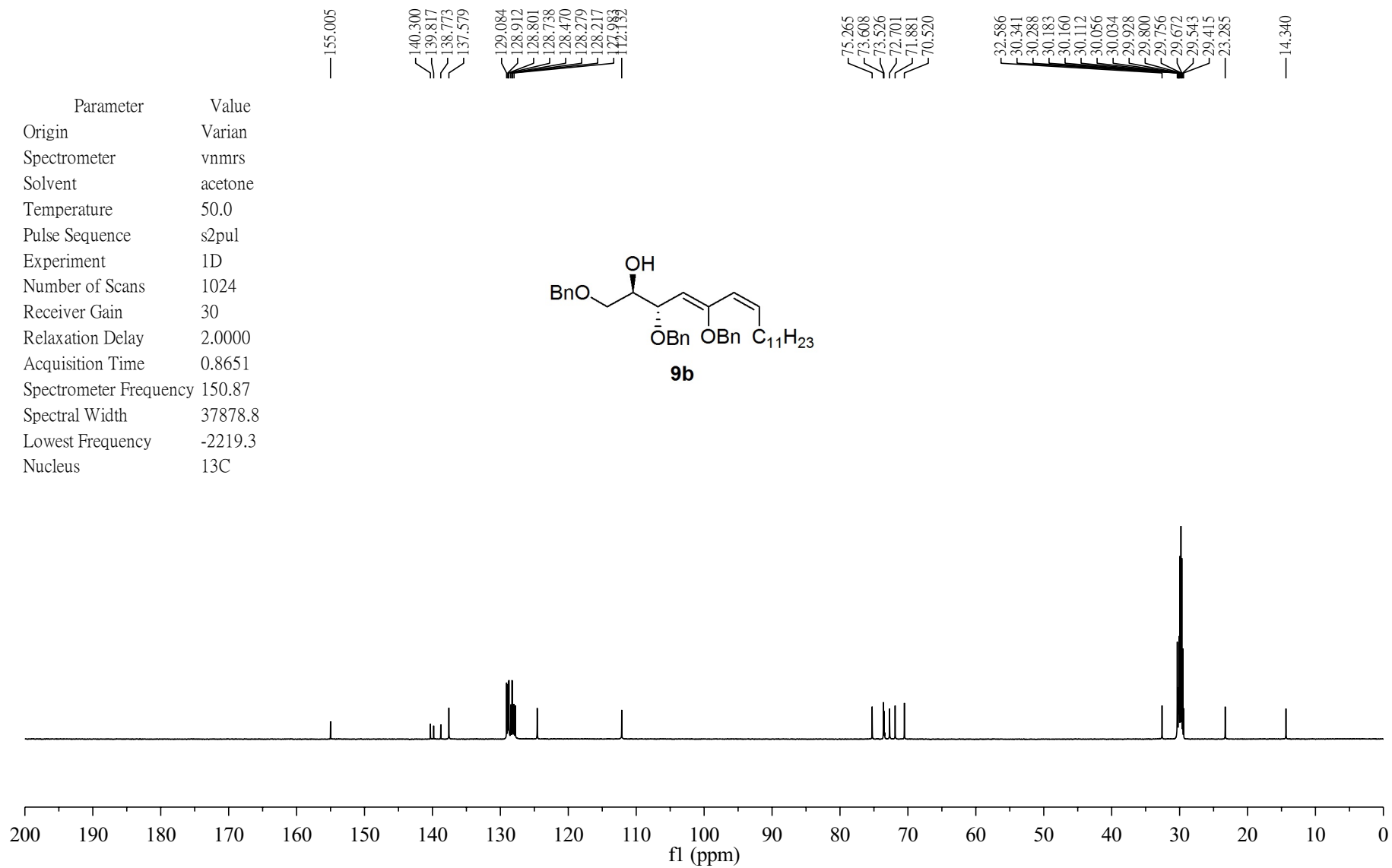
Parameter	Value (f2, f1)
Origin	Varian
Spectrometer	vnmrs
Solvent	cdcl3
Temperature	9.0
Pulse Sequence	gCOSY
Experiment	2D-COSY
Number of Scans	1
Receiver Gain	30
Relaxation Delay	1.0000
Acquisition Time	0.1501
Spectrometer Frequency	(399.76, 399.76)
Spectral Width	(6410.3, 6410.3)
Lowest Frequency	(-798.5, -804.5)
Nucleus	(1H, 1H)
Acquired Size	(962, 128)
Spectral Size	(1024, 1024)

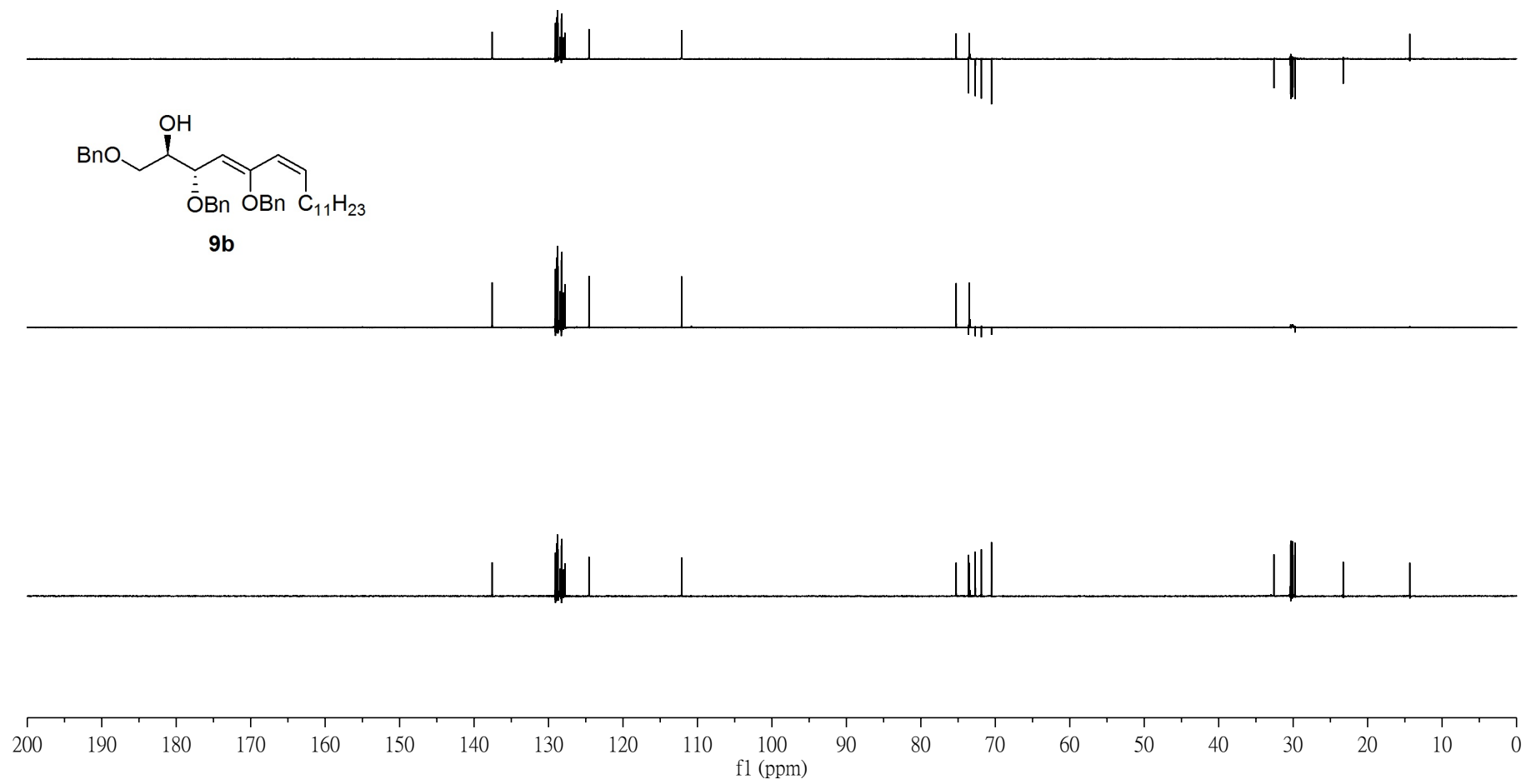


Parameter	Value (f2, f1)
Origin	Varian
Spectrometer	vnmrs
Solvent	cdcl3
Temperature	9.0
Pulse Sequence	gHSQC
Experiment	2D-HSQC-EDITED
Number of Scans	4
Receiver Gain	30
Relaxation Delay	1.0000
Acquisition Time	0.1501
Spectrometer Frequency	(399.76, 100.53)
Spectral Width	(6410.3, 17086.7)
Lowest Frequency	(-799.9, -1009.6)
Nucleus	(1H, 13C)
Acquired Size	(962, 128)
Spectral Size	(1024, 1024)



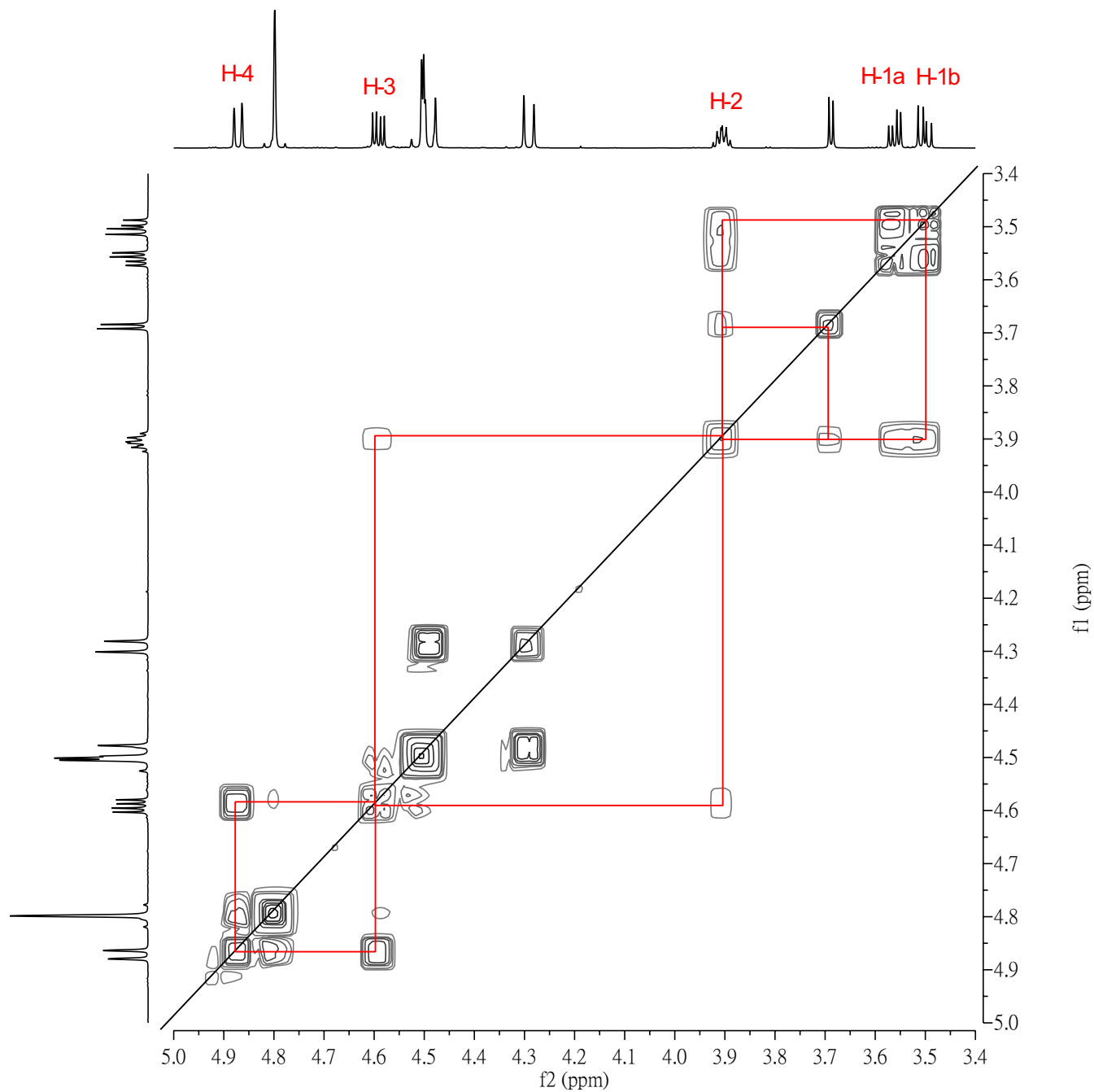
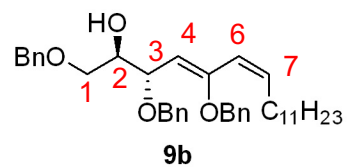




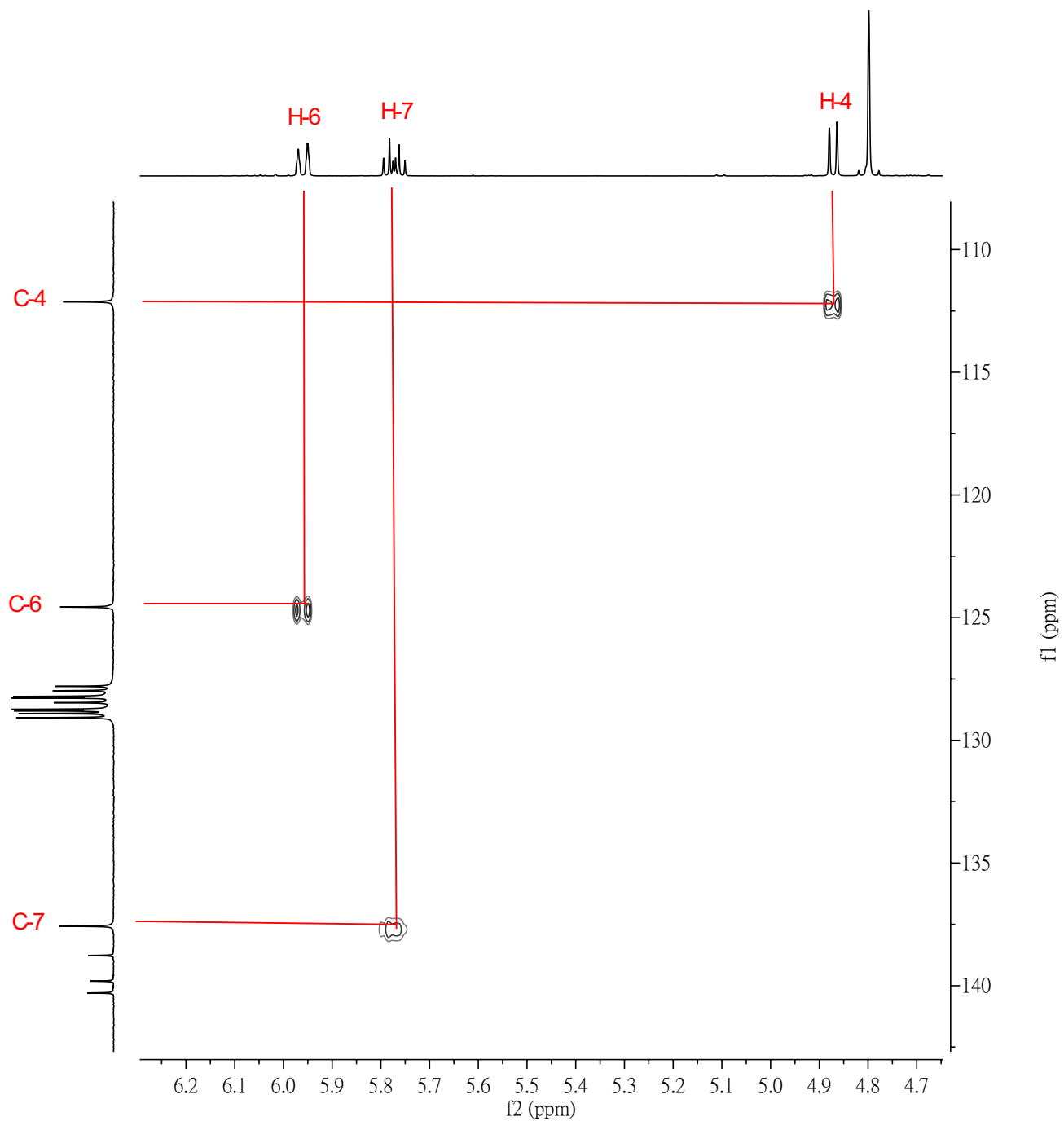
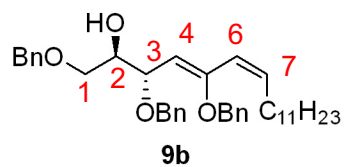


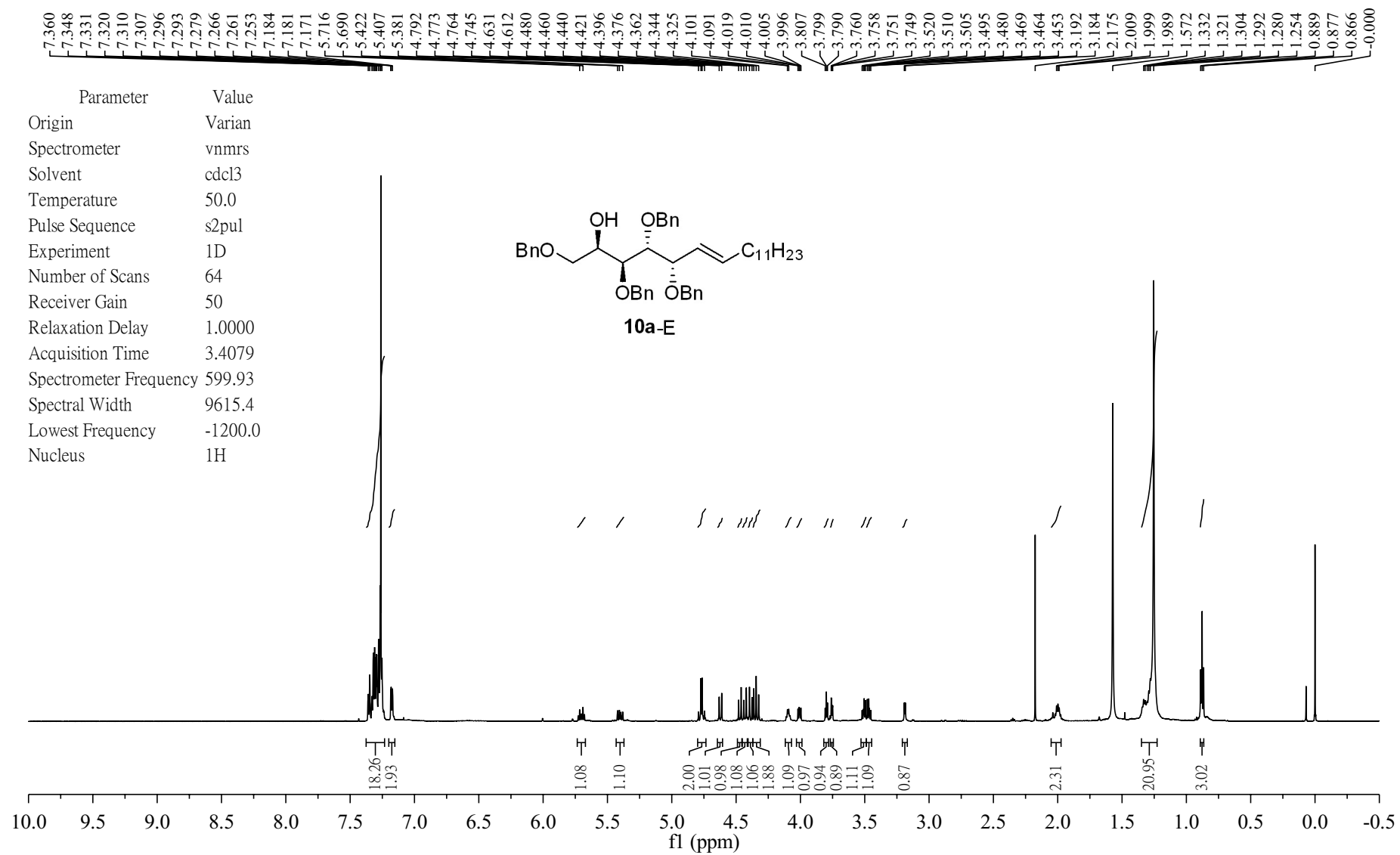


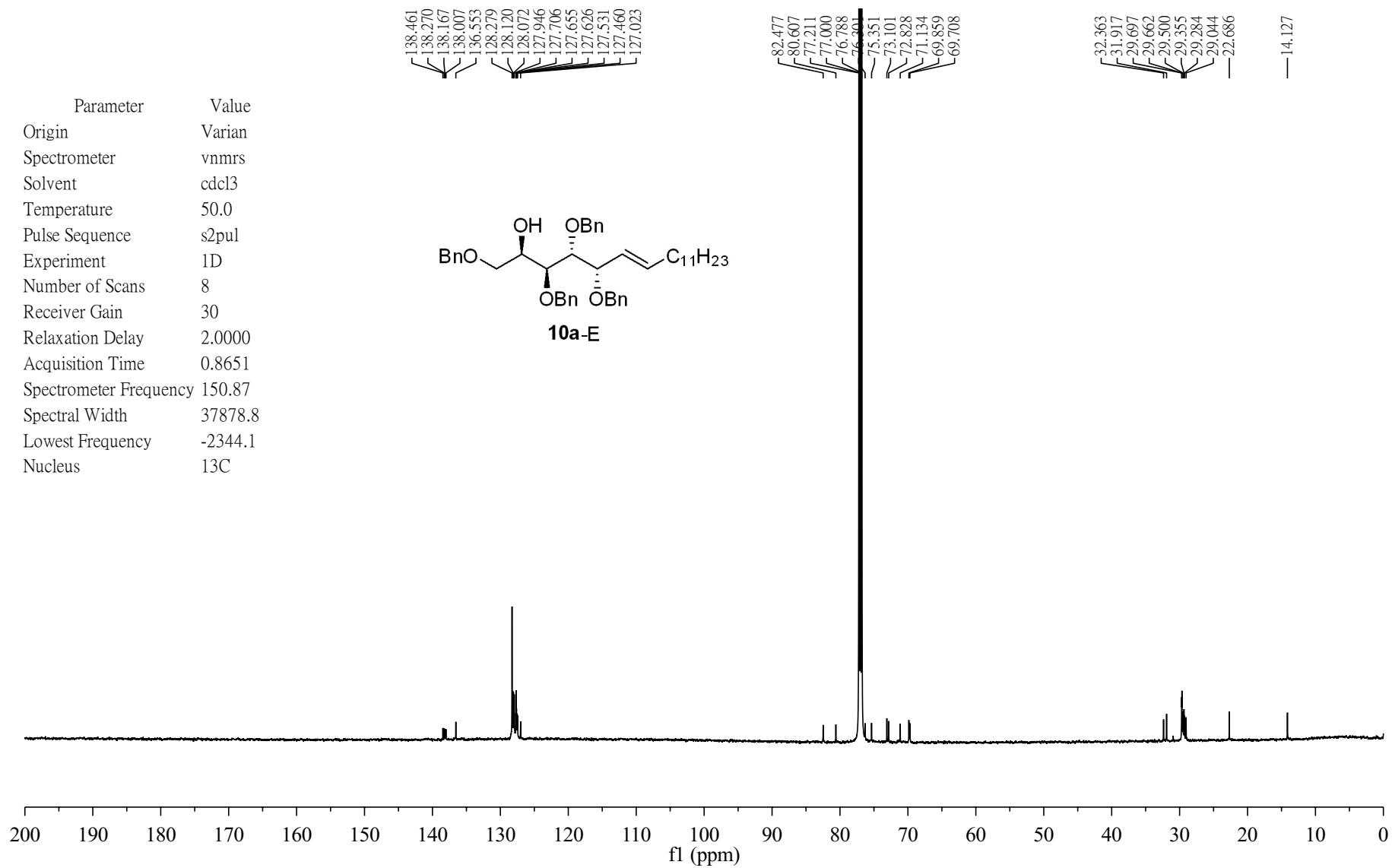
Parameter	Value (f2, f1)
Origin	Varian
Spectrometer	nmrs
Solvent	acetone
Temperature	50.0
Pulse Sequence	gCOSY
Experiment	2D-COSY
Number of Scans	16
Receiver Gain	30
Relaxation Delay	1.0000
Acquisition Time	0.1500
Spectrometer Frequency	(599.94, 599.94)
Spectral Width	(9615.4, 9615.4)
Lowest Frequency	(-1200.9, -1205.8)
Nucleus	(1H, 1H)
Acquired Size	(1442, 256)
Spectral Size	(2048, 2048)

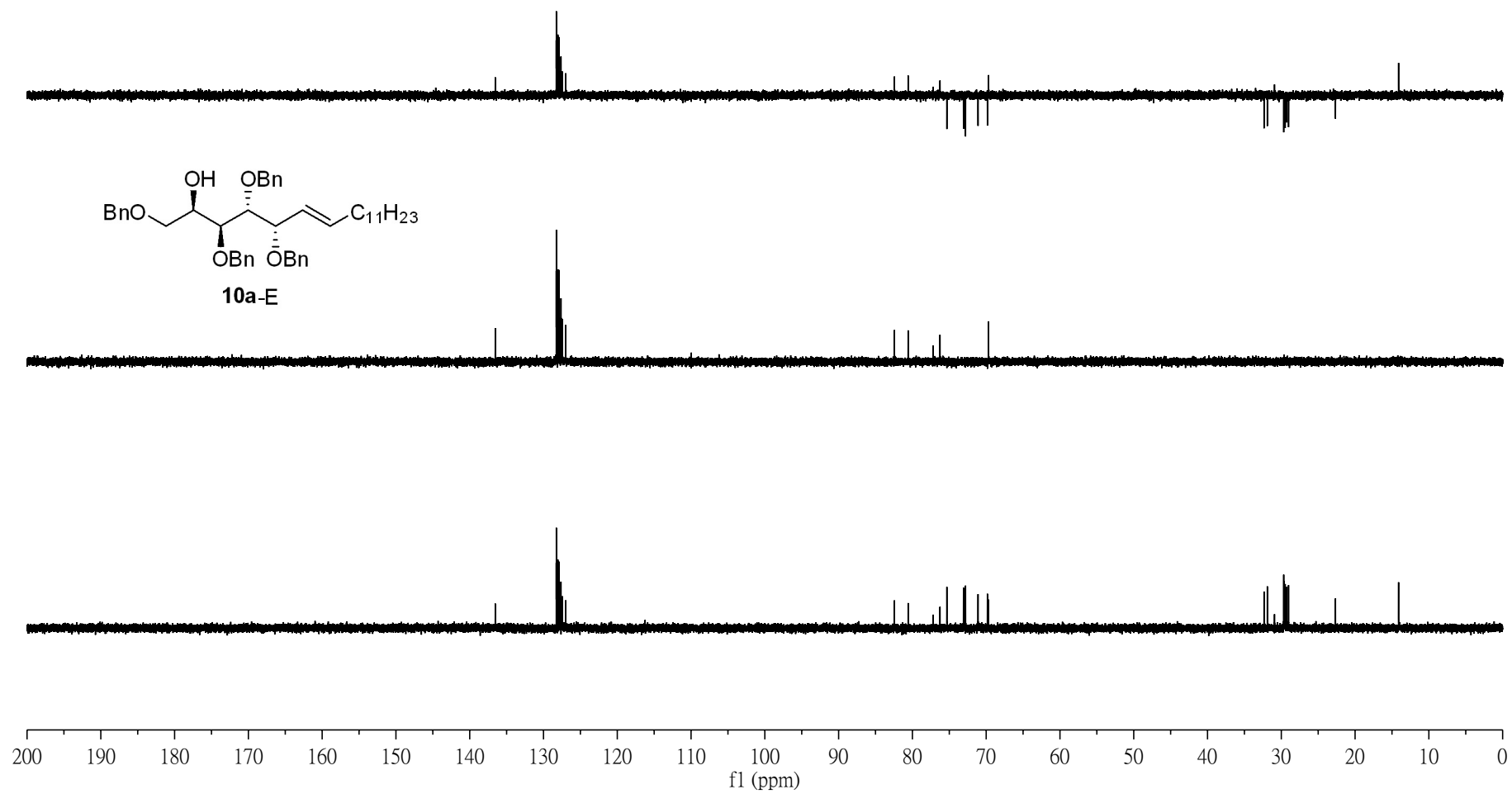


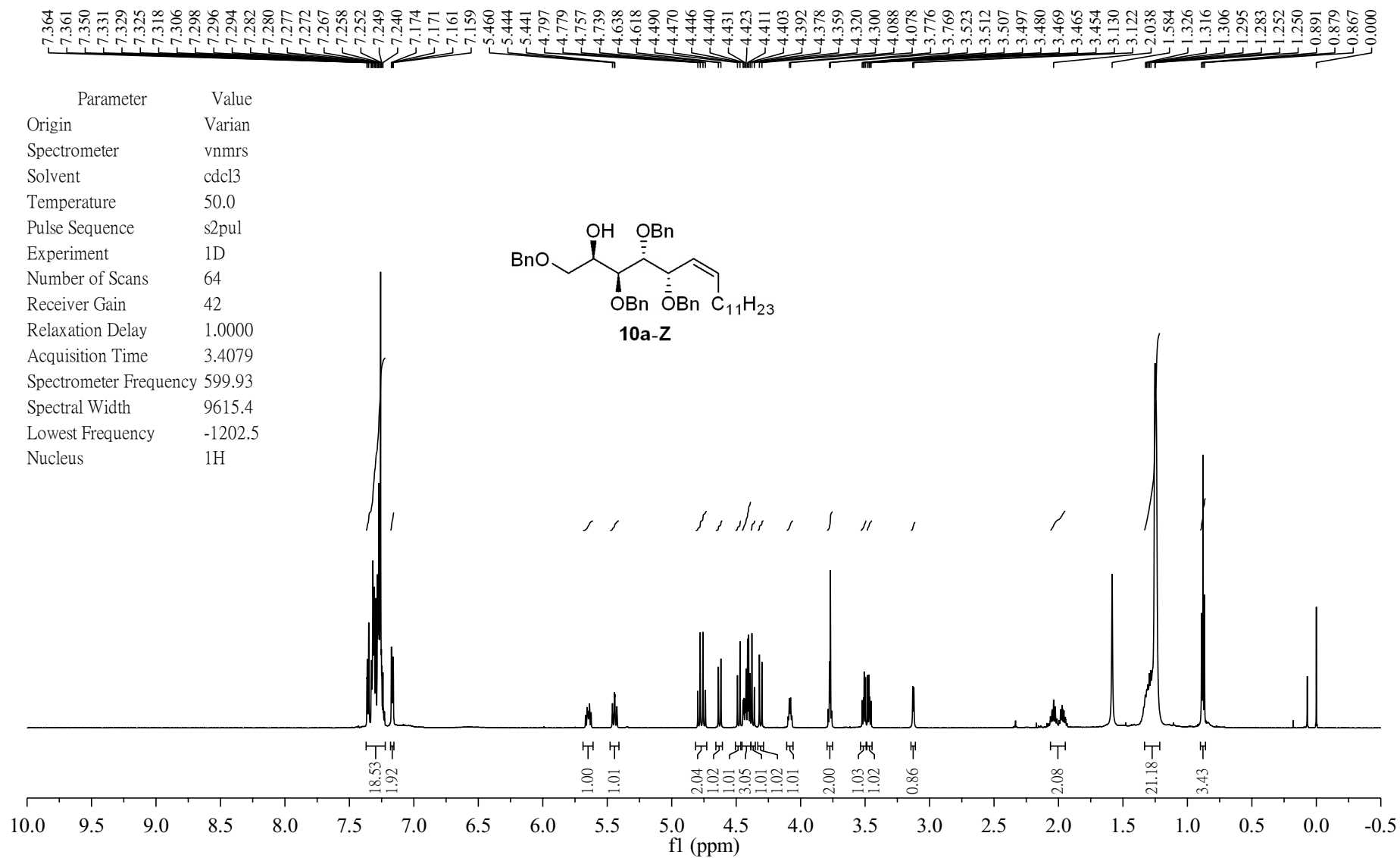
Parameter	Value (f2, f1)
Origin	Varian
Spectrometer	vnmrs
Solvent	acetone
Temperature	50.0
Pulse Sequence	gHSQCAD
Experiment	2D-HSQC-EDITED
Number of Scans	32
Receiver Gain	30
Relaxation Delay	1.0000
Acquisition Time	0.1500
Spectrometer Frequency (599.94, 150.87)	
Spectral Width	(9615.4, 30165.9)
Lowest Frequency	(-1200.9, -1361.9)
Nucleus	(1H, 13C)
Acquired Size	(1442, 256)
Spectral Size	(2048, 2048)

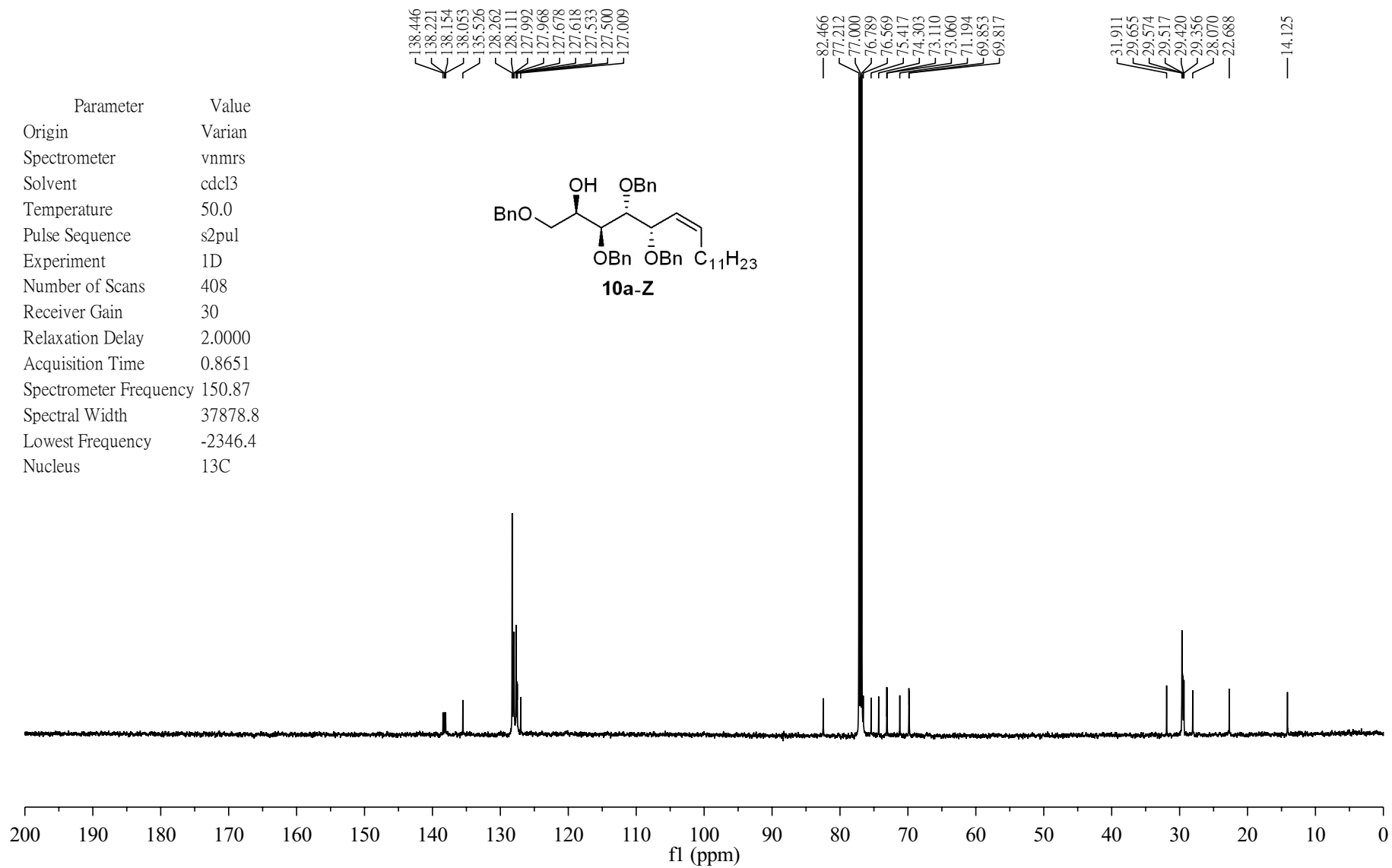


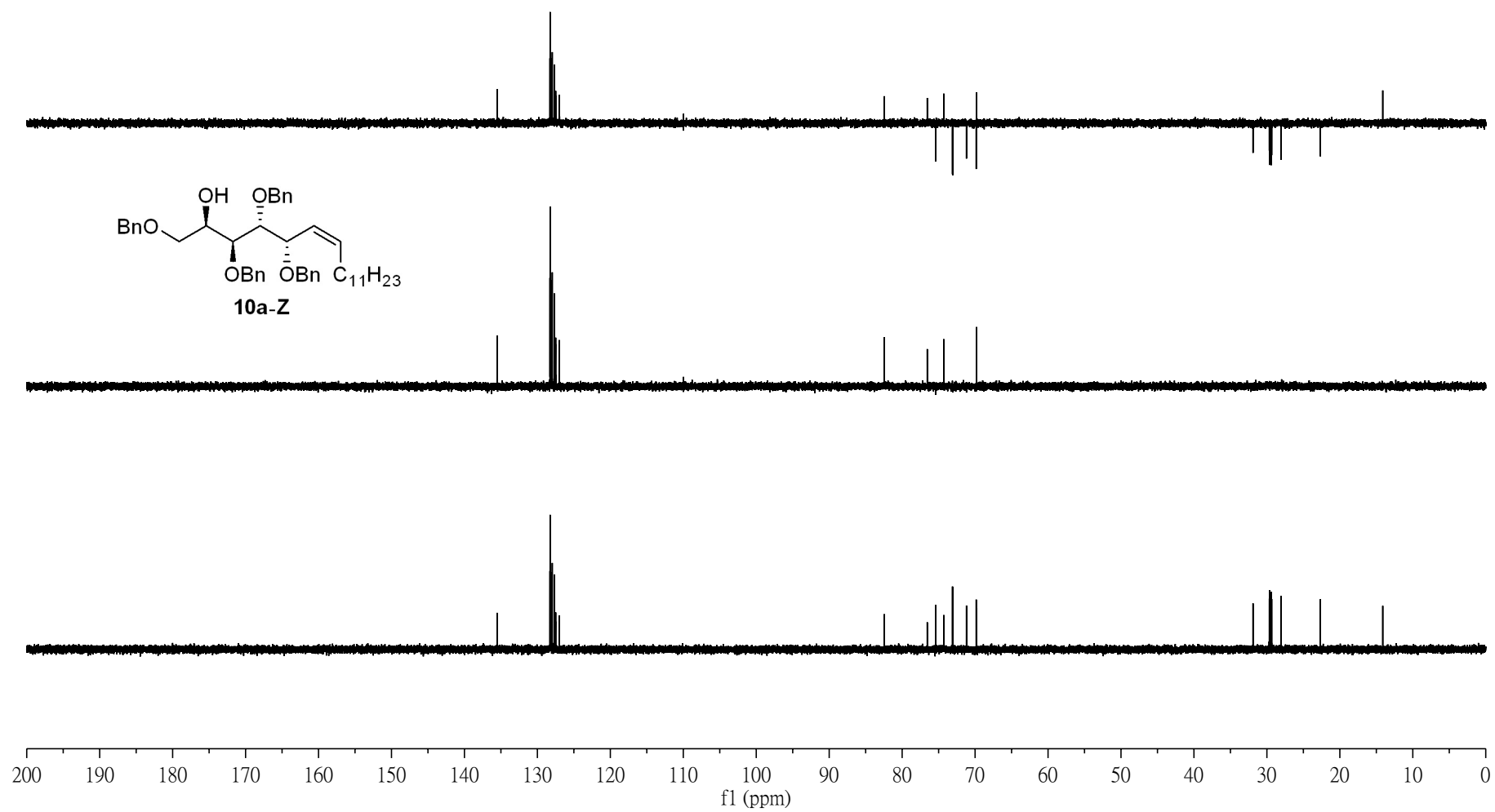




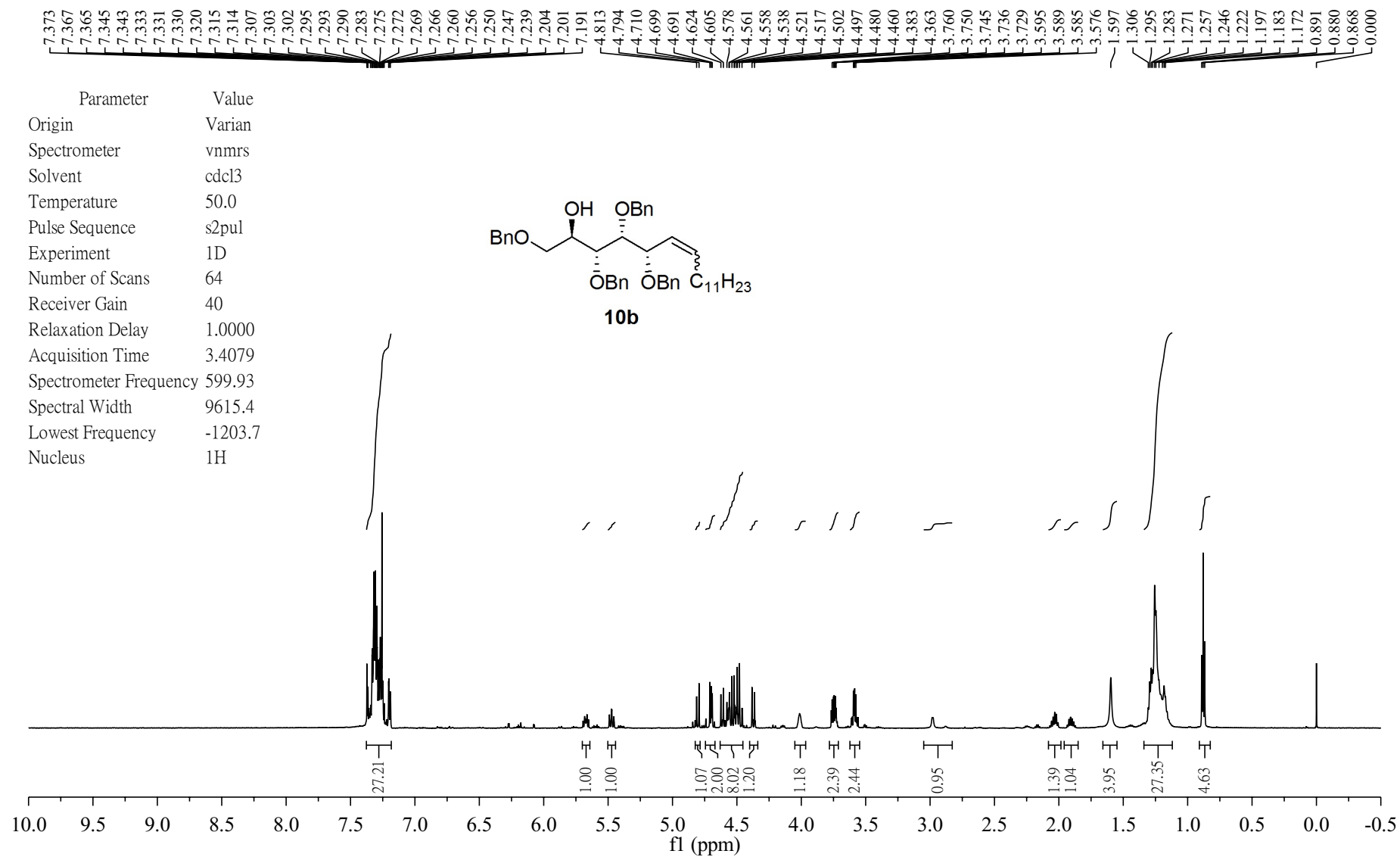


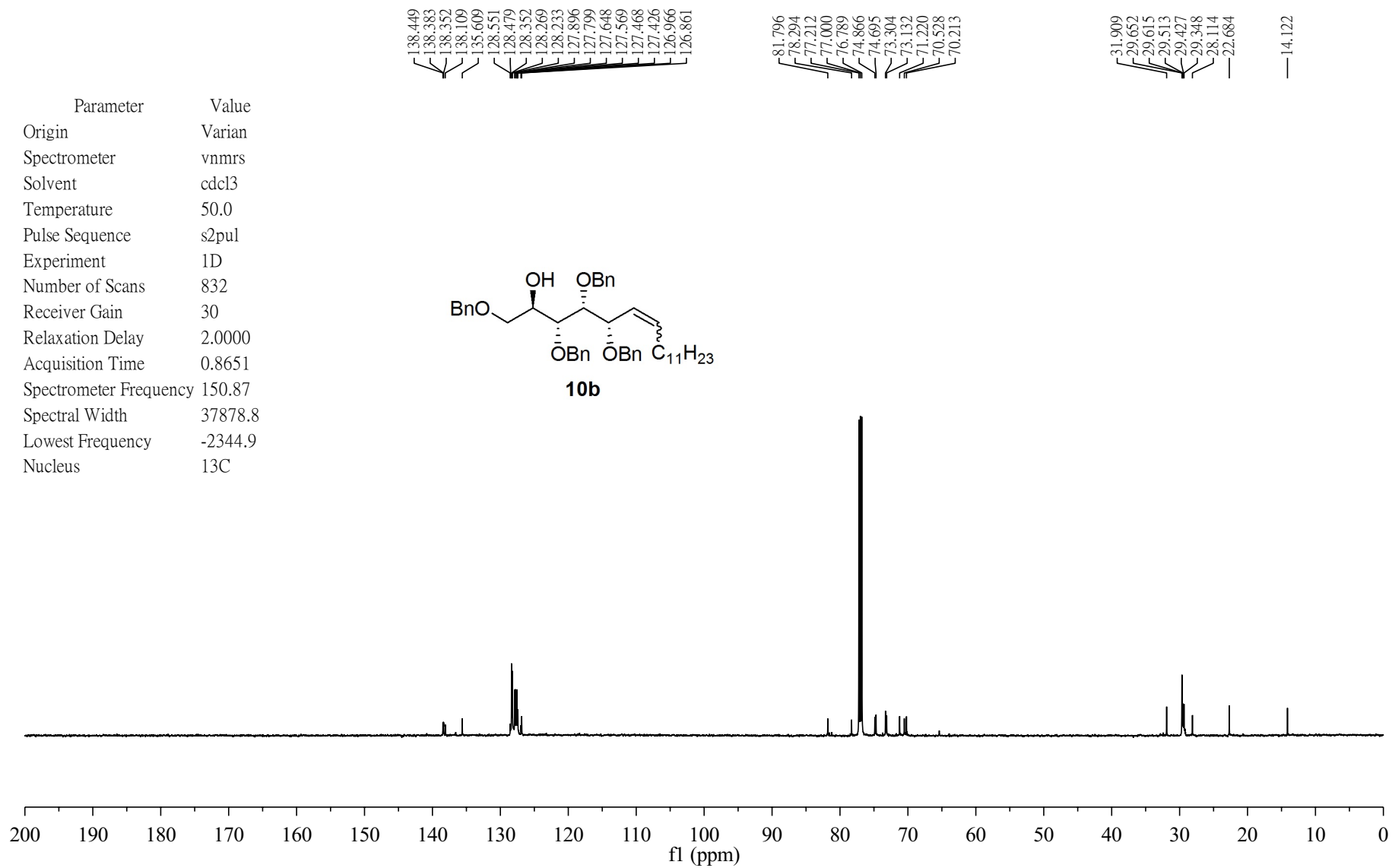


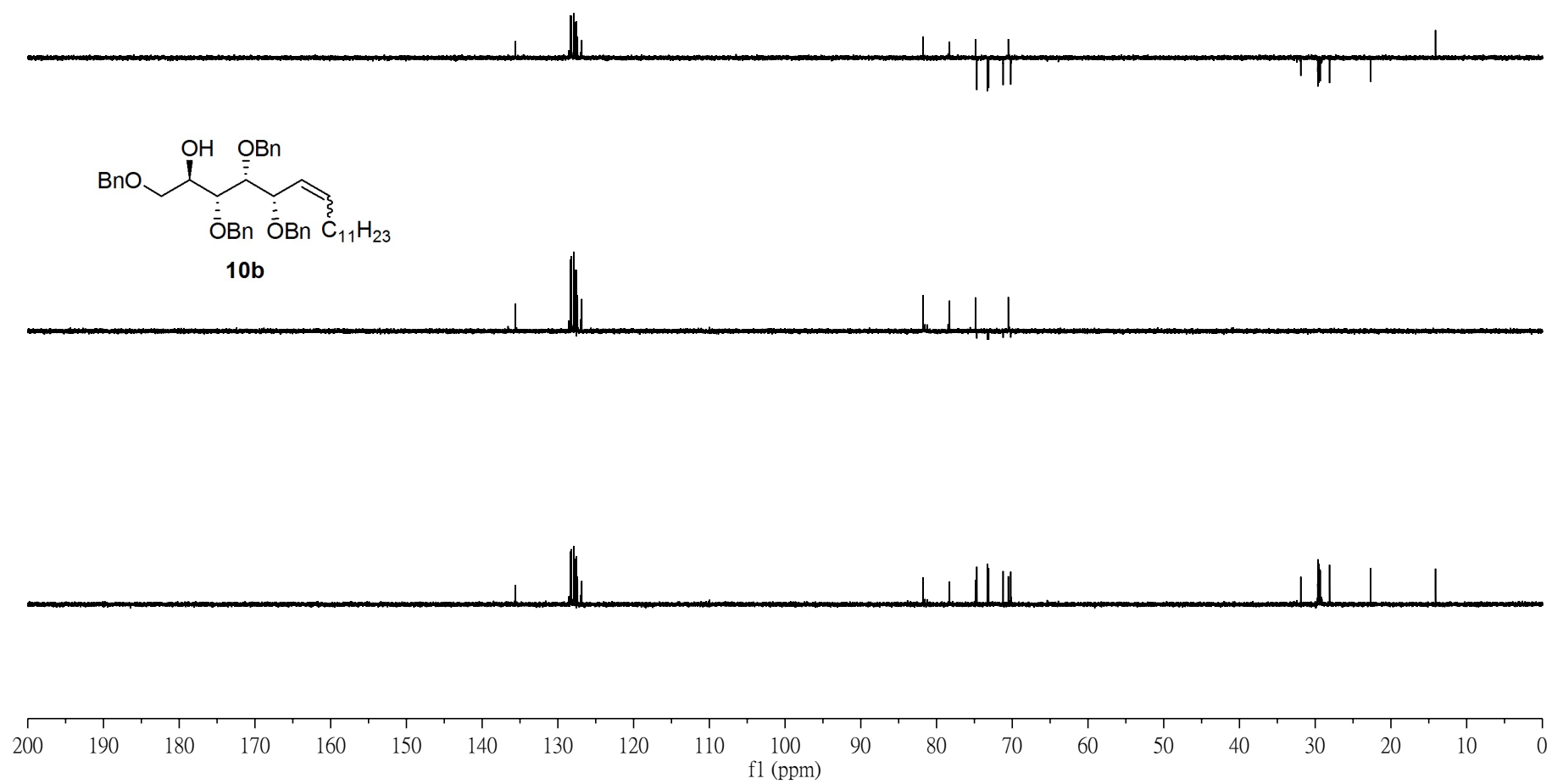


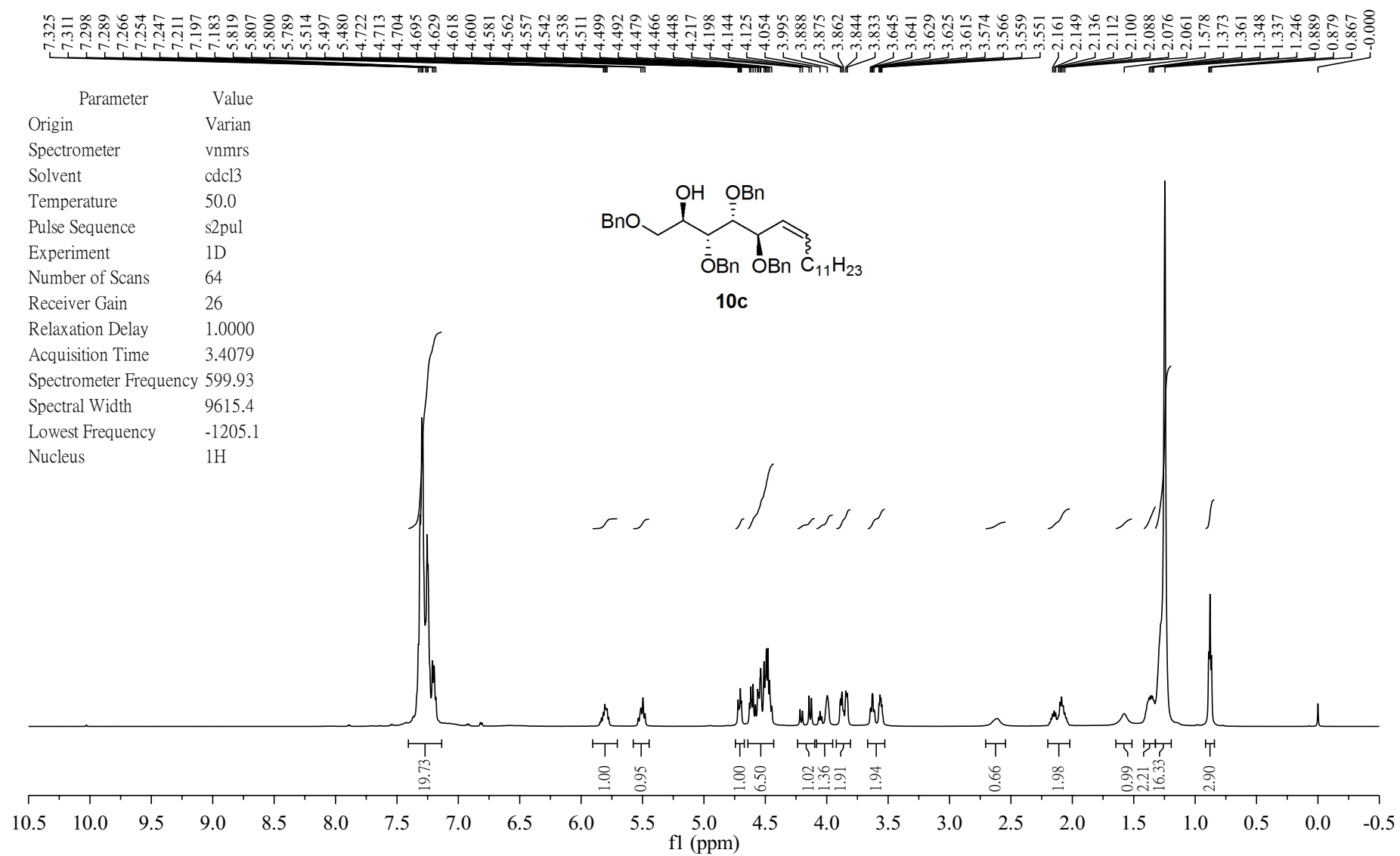


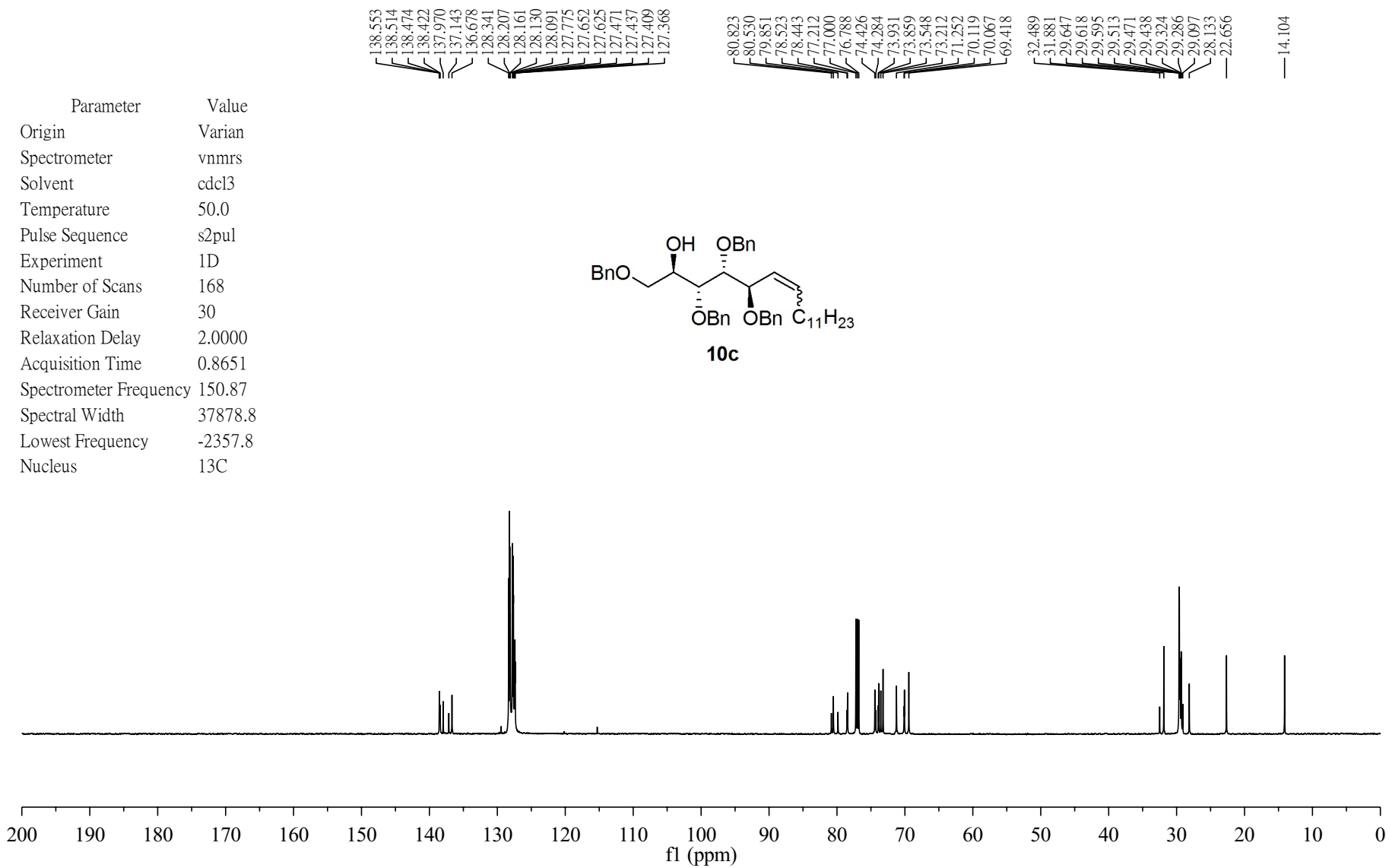


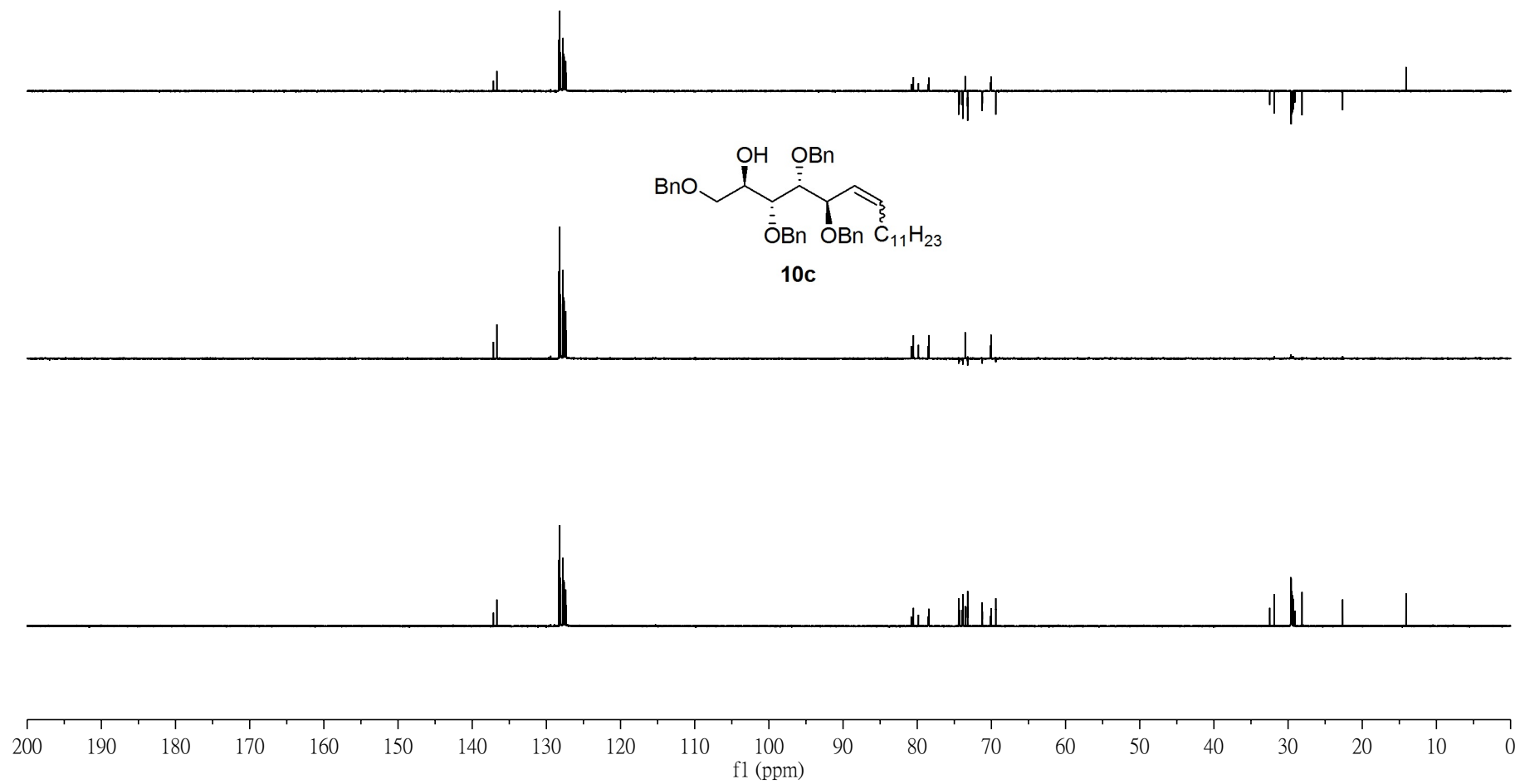


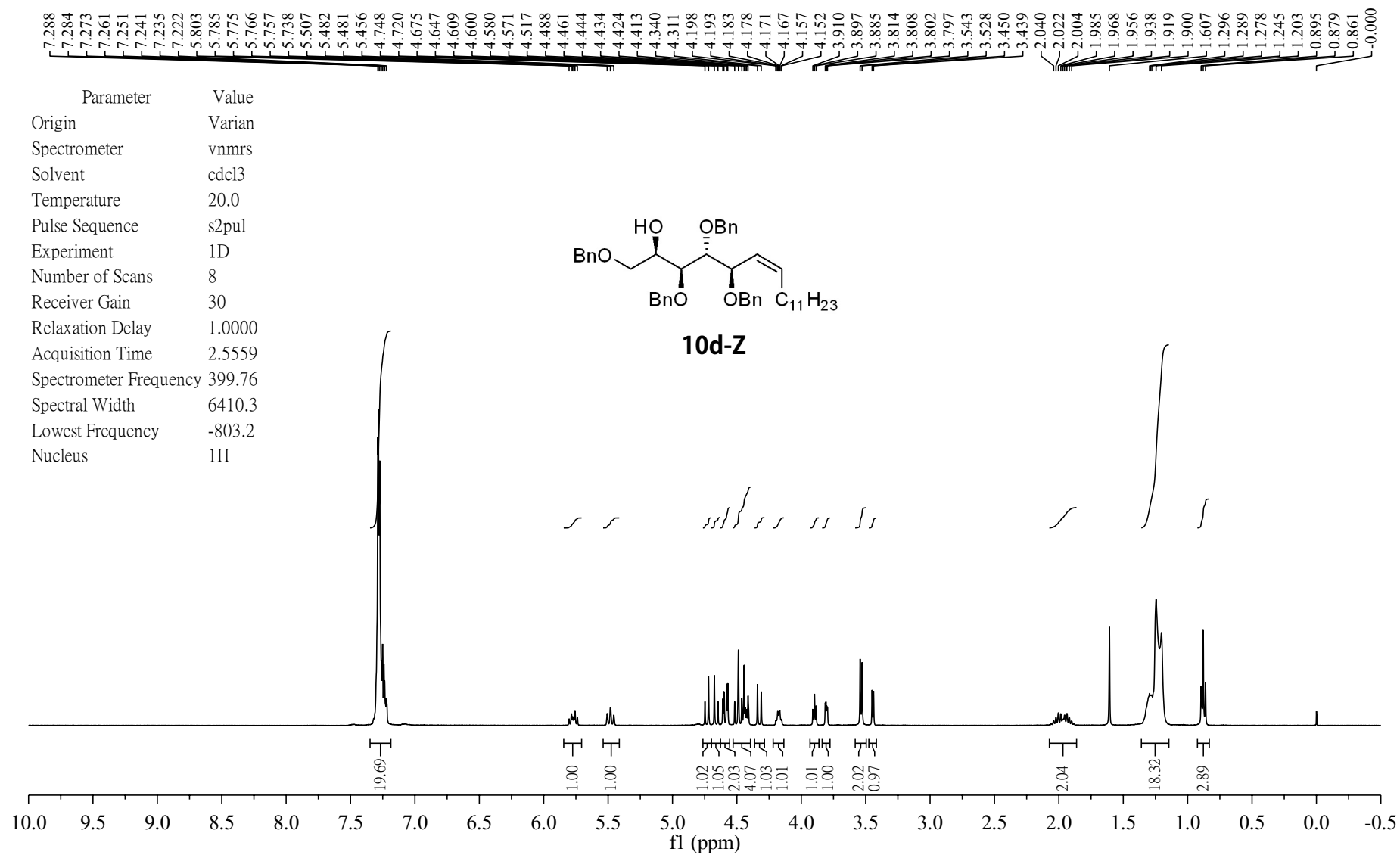


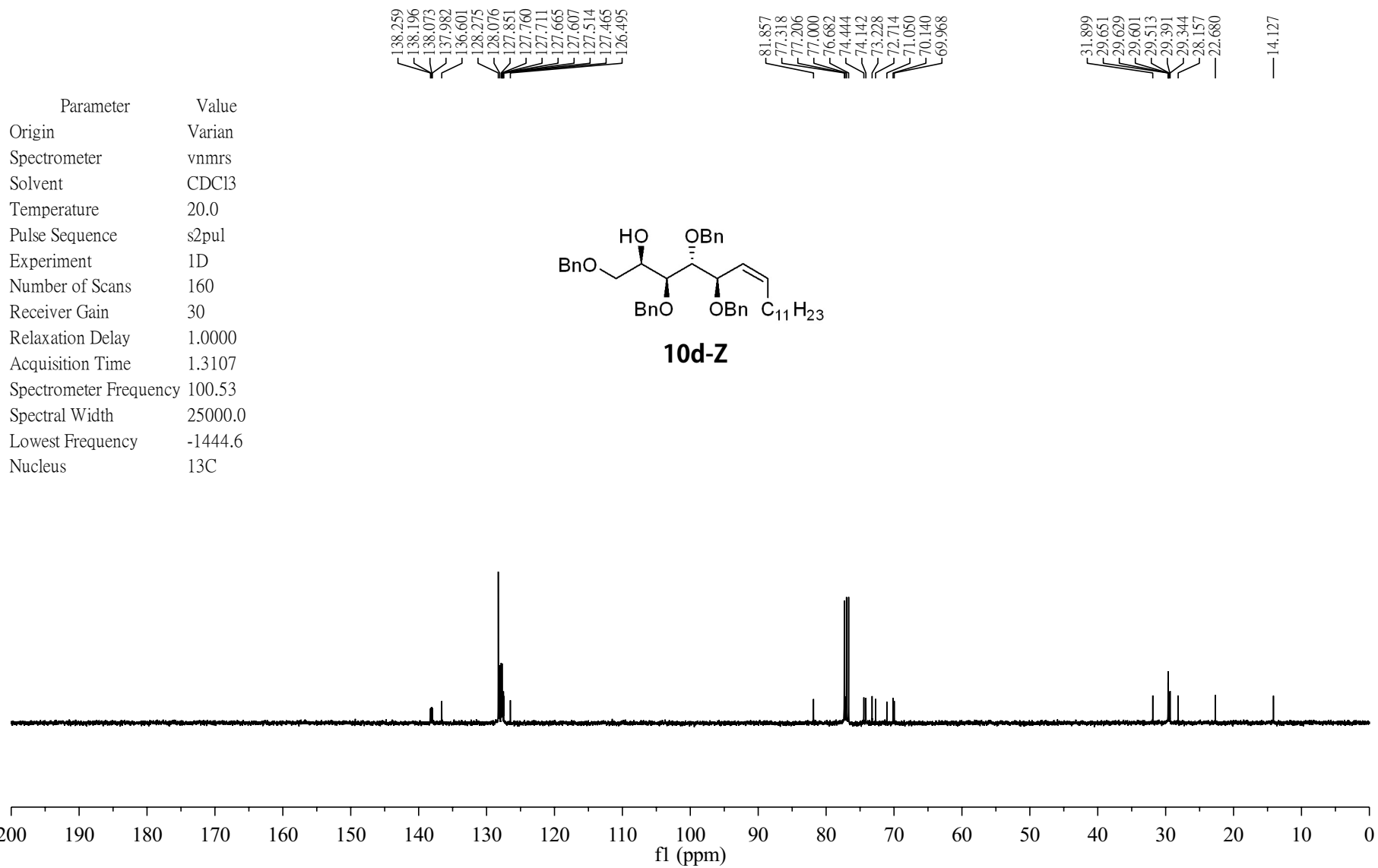




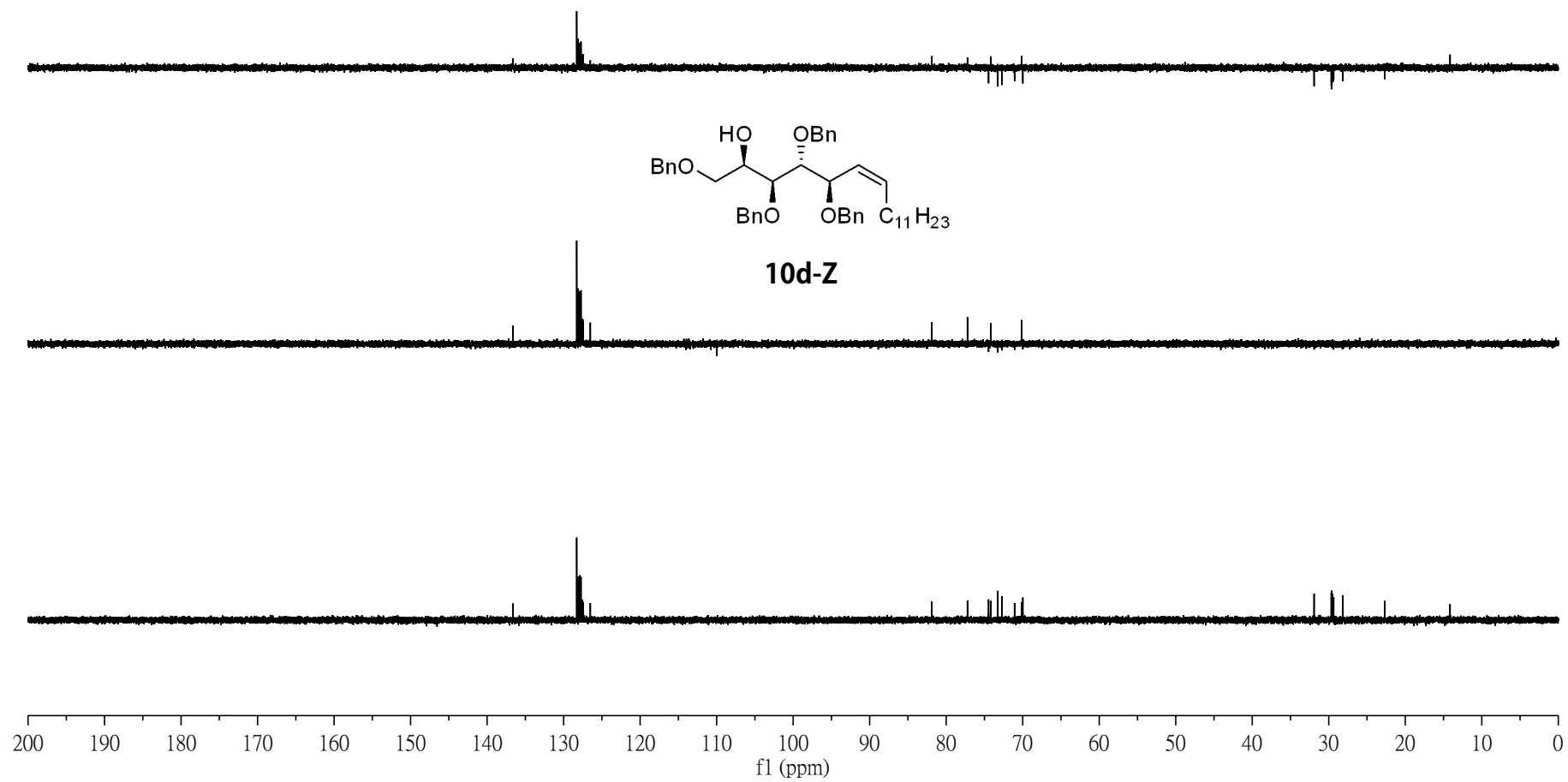


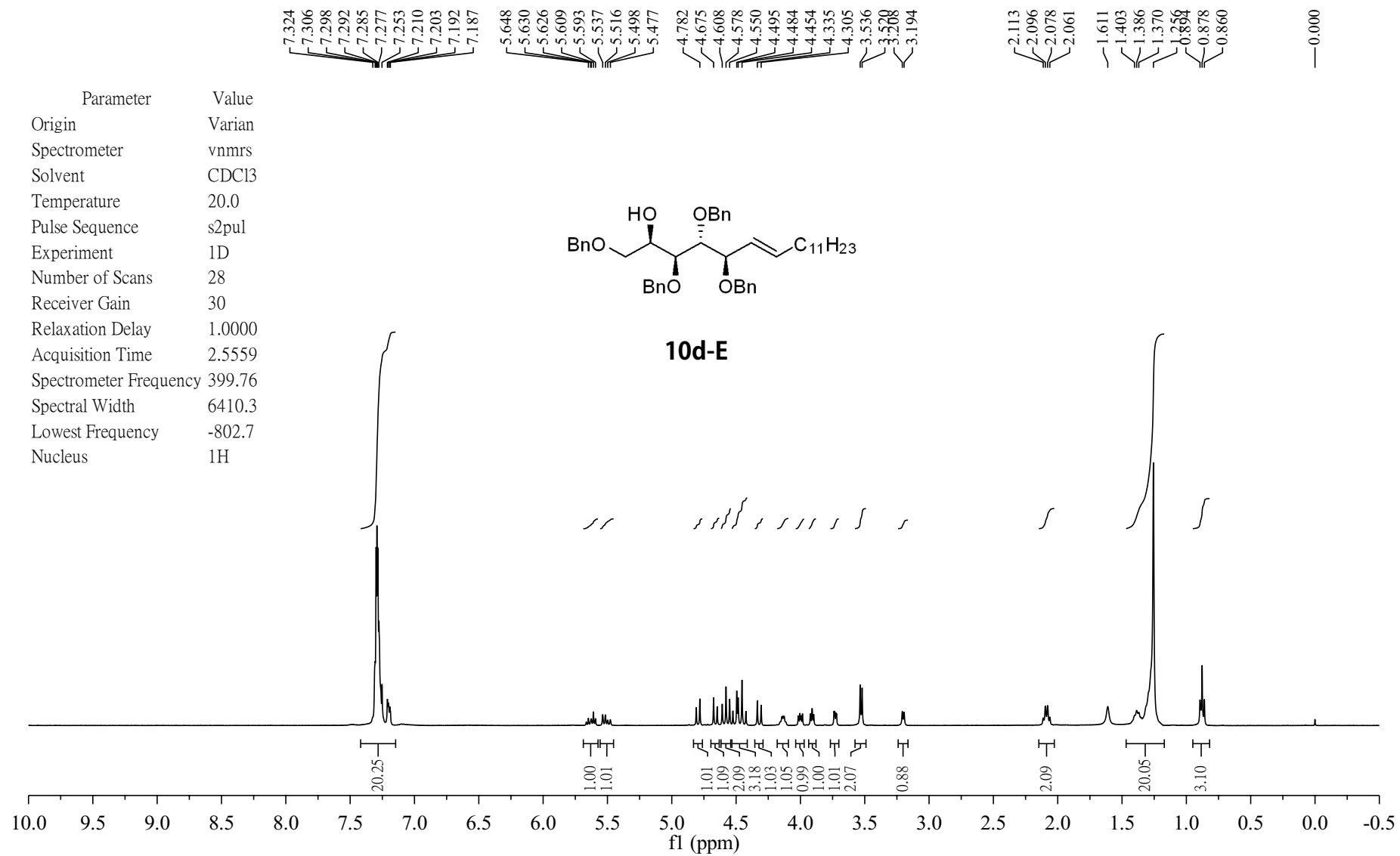


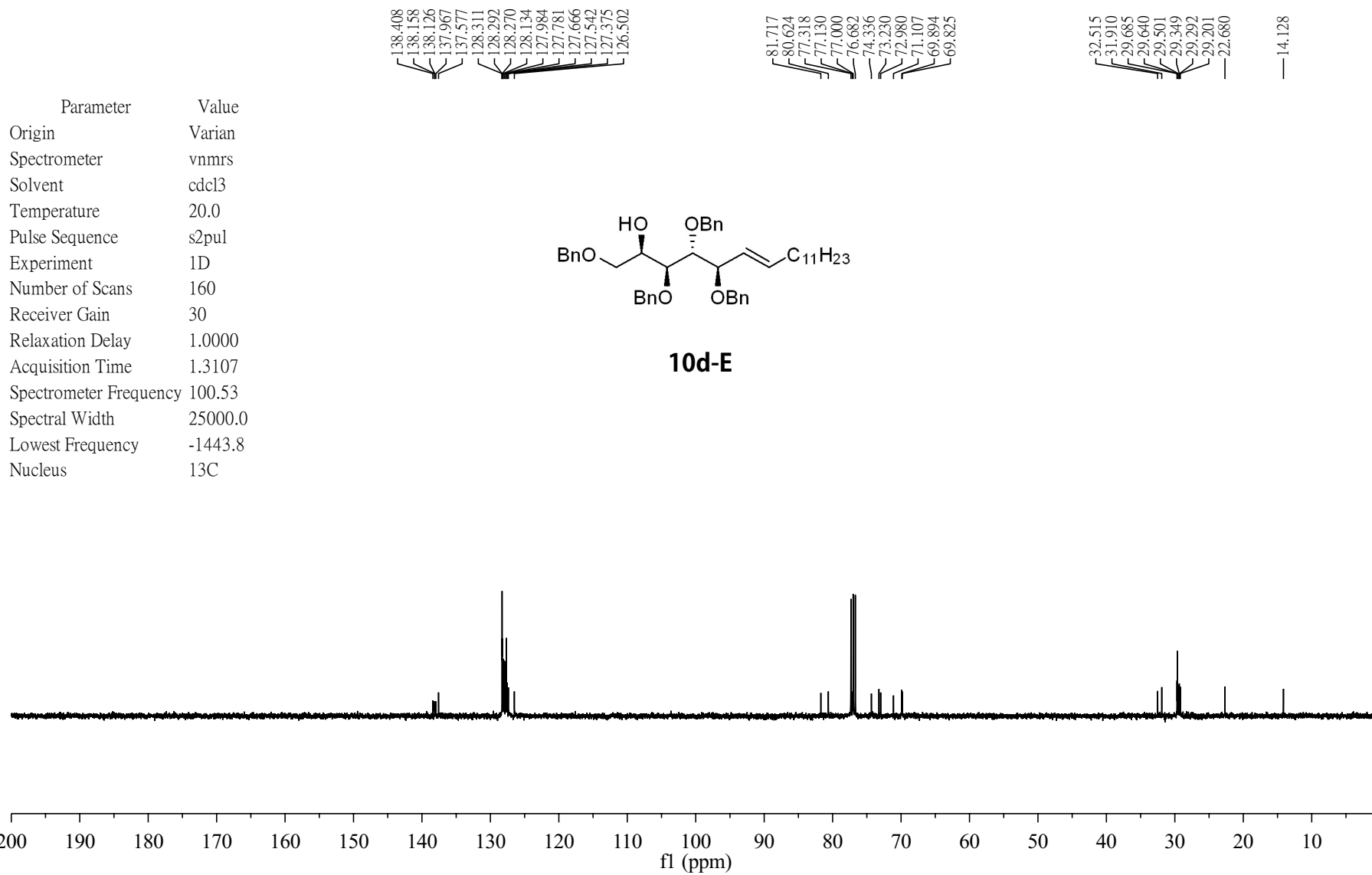


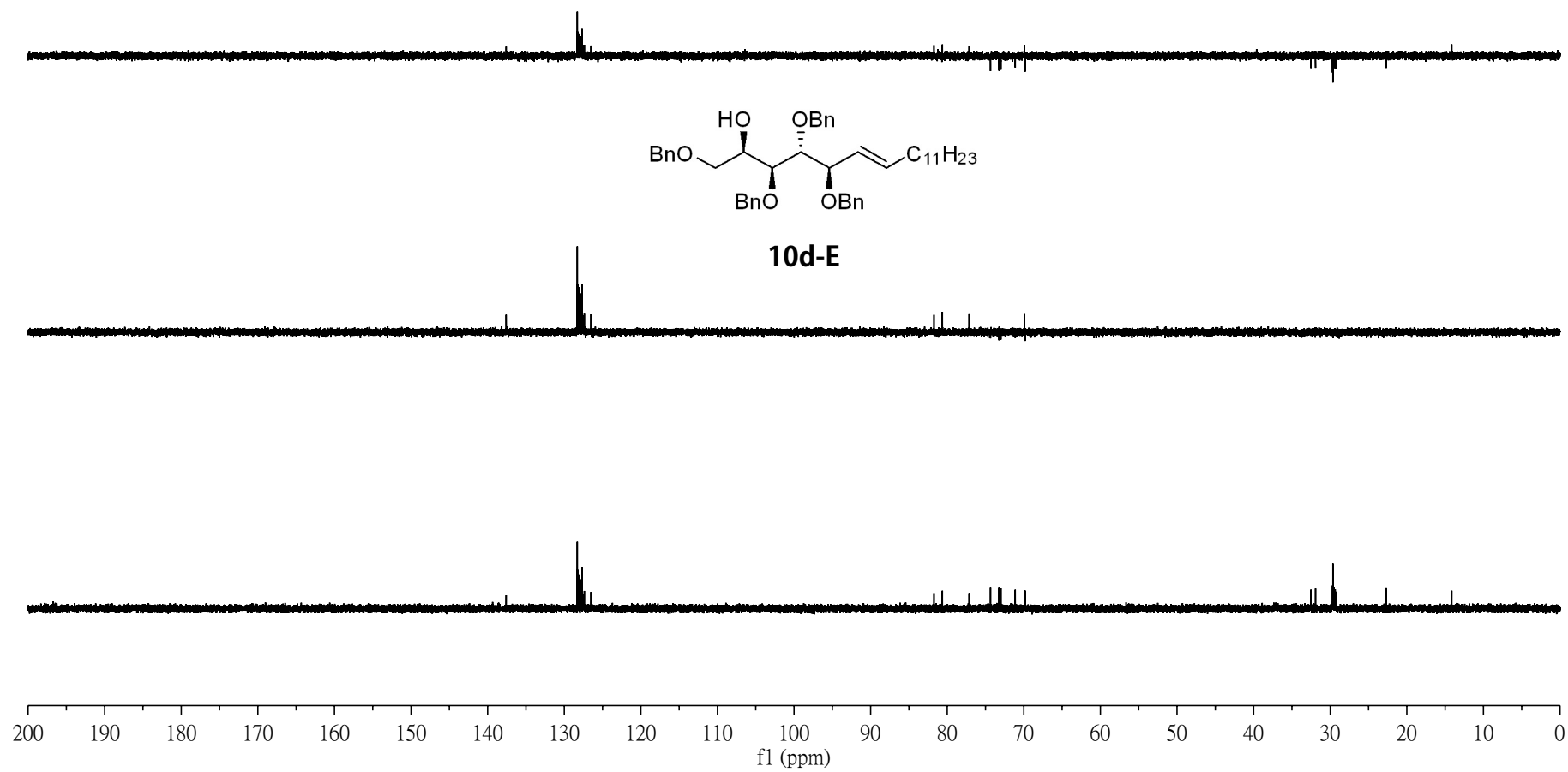




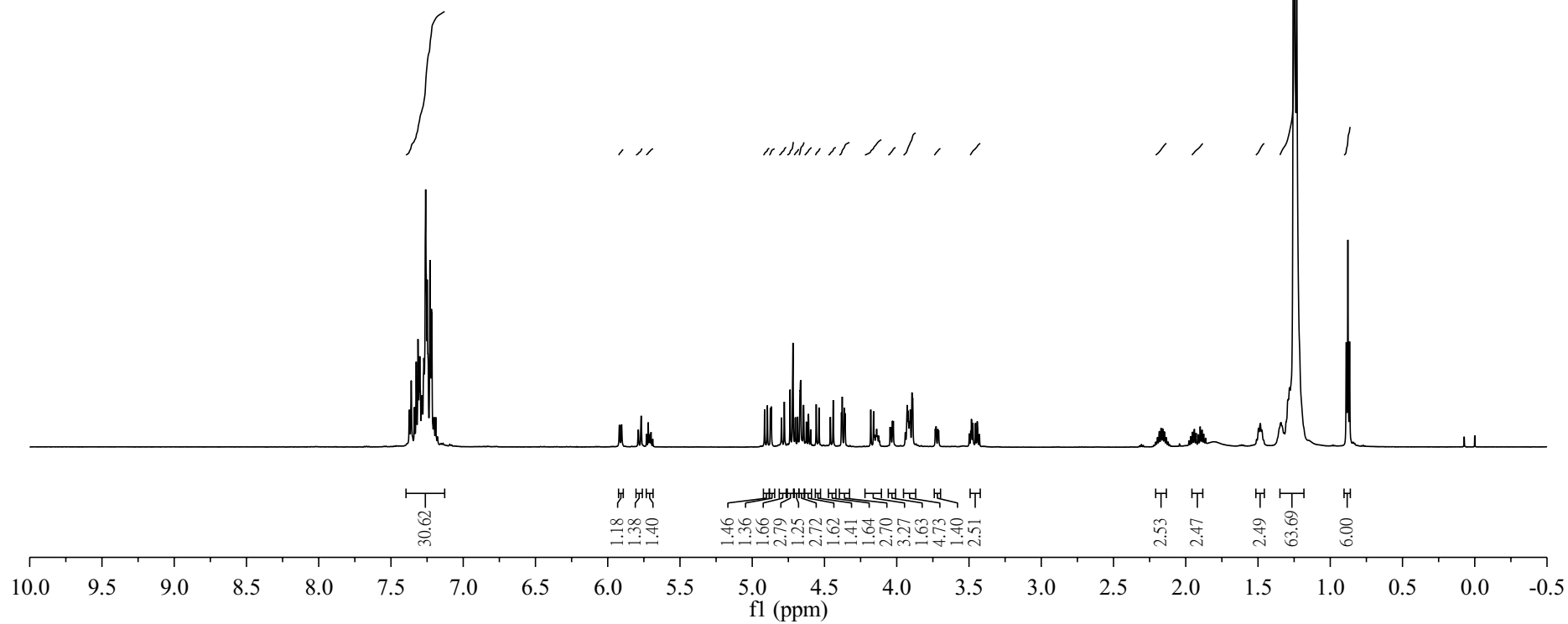
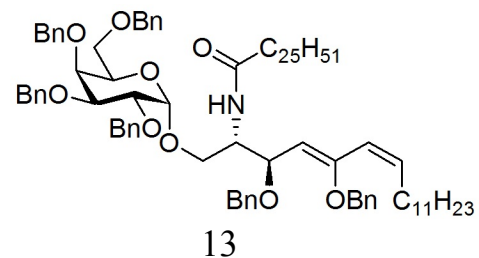




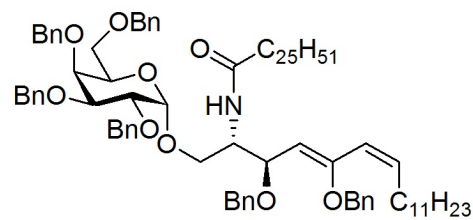




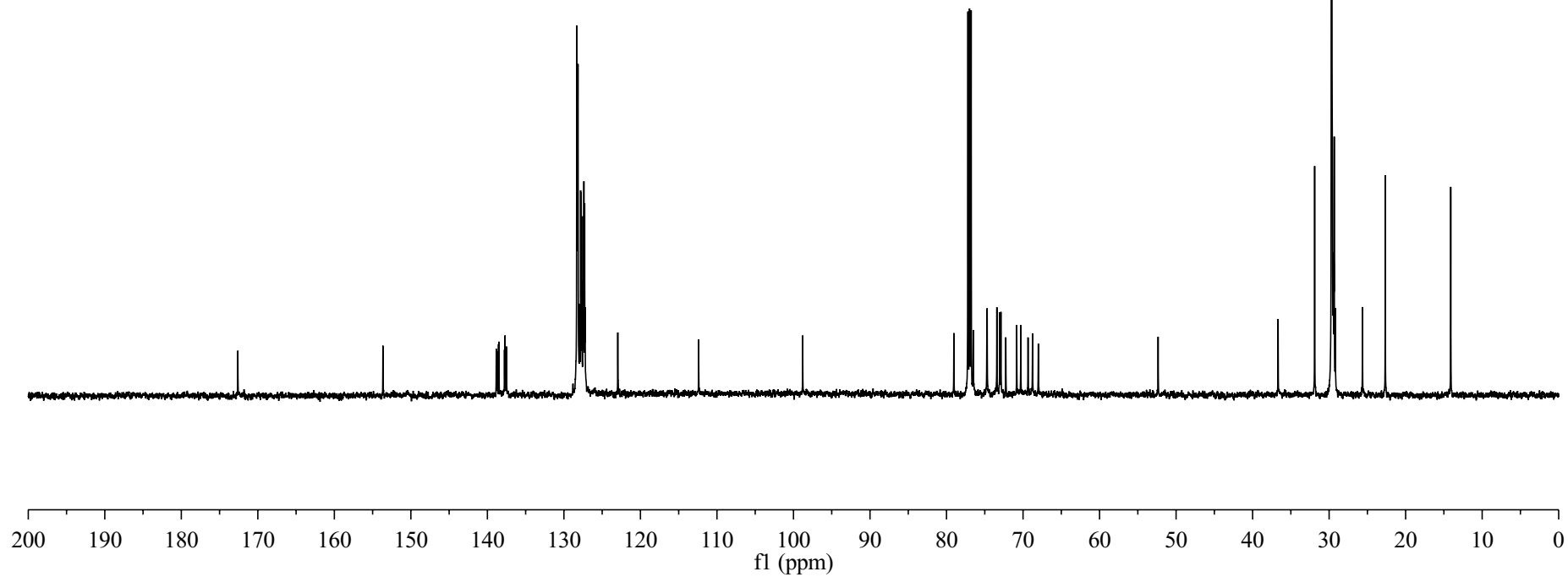
Parameter	Value
1 Comment	HSL-261
2 Origin	Varian
3 Spectrometer	inova
4 Author	vnmr1
5 Solvent	CDCl3
6 Temperature	29.0
7 Pulse Sequence	s2pul
8 Number of Scans	64
9 Receiver Gain	30
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	2.0000
13 Modification Date	2012-08-29T16:43:26
14 Spectrometer Frequency	599.94
15 Spectral Width	8000.0
16 Lowest Frequency	-500.0
17 Nucleus	1H
18 Acquired Size	16000
19 Spectral Size	32768



Parameter	Value
1 Comment	HSL-261
2 Origin	Varian
3 Spectrometer	inova
4 Author	vnmr1
5 Solvent	CDC13
6 Temperature	22.0
7 Pulse Sequence	s2pul
8 Number of Scans	256
9 Receiver Gain	58
10 Relaxation Delay	0.5000
11 Pulse Width	0.0000
12 Acquisition Time	0.9997
13 Modification Date	2012-08-29T16:43:22
14 Spectrometer Frequency	150.87
15 Spectral Width	40000.0
16 Lowest Frequency	-4043.5
17 Nucleus	$^{13}\text{C}$
18 Acquired Size	39987
19 Spectral Size	131072

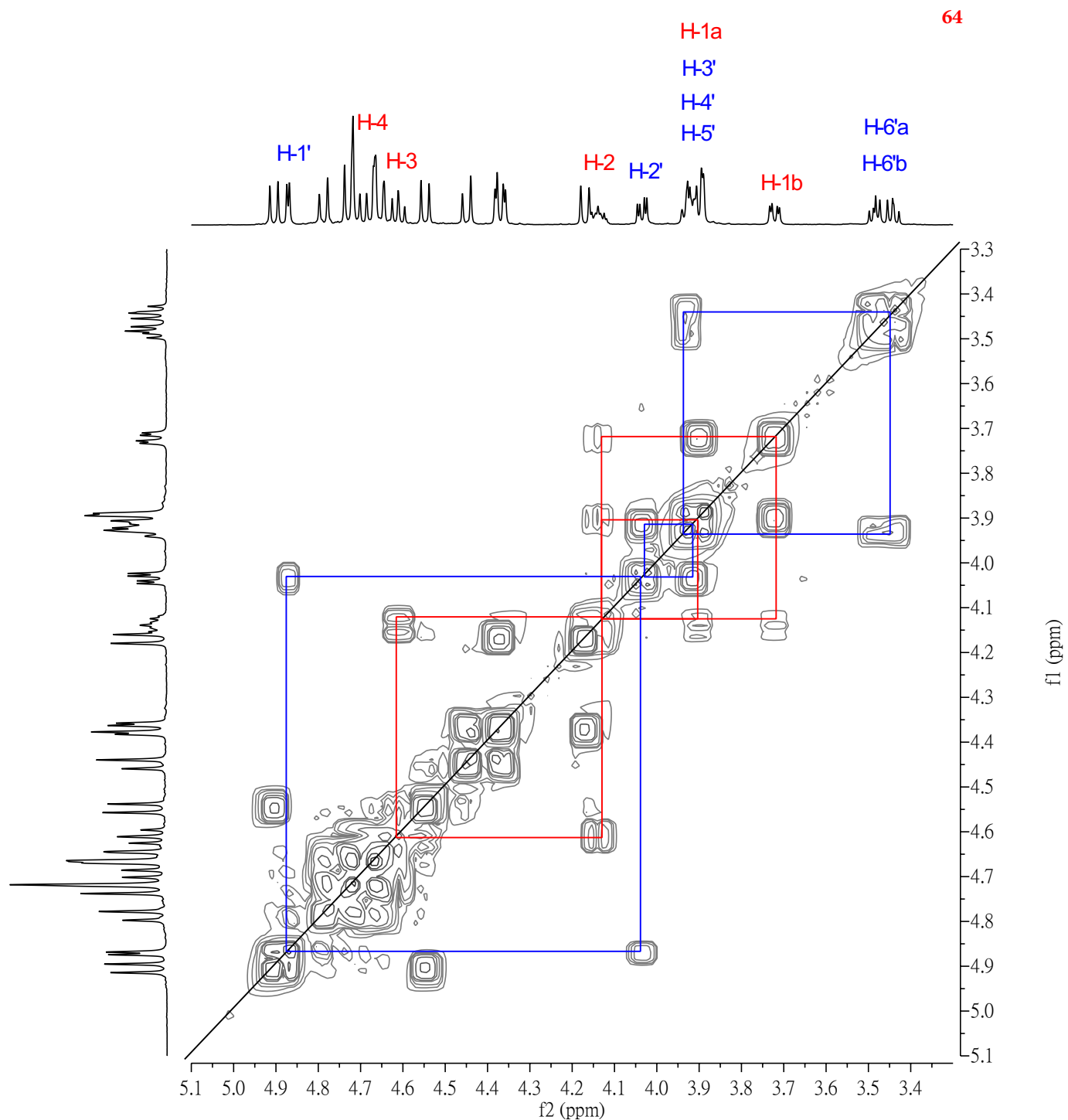
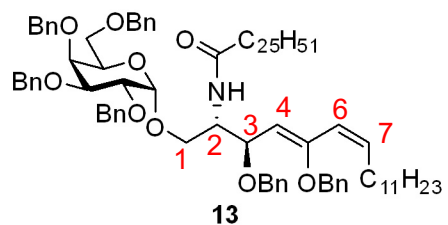


13



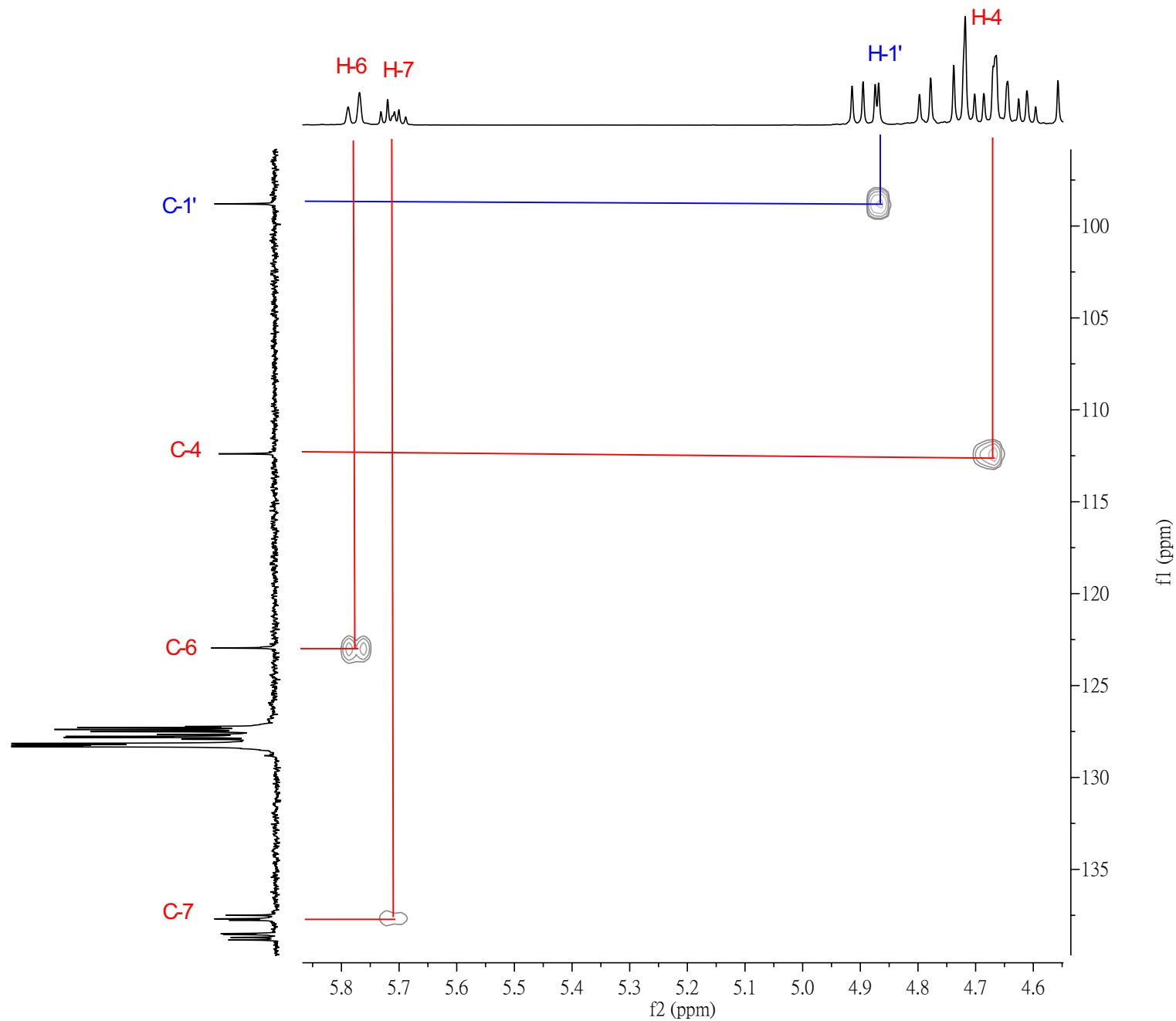
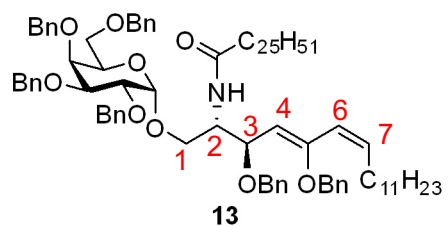


Parameter	Value (f2, f1)
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	29.0
Pulse Sequence	gCOSY
Experiment	2D-COSY
Number of Scans	16
Receiver Gain	30
Relaxation Delay	1.0000
Acquisition Time	0.1280
Spectrometer Frequency	(599.94, 599.94)
Spectral Width	(8000.0, 8000.0)
Lowest Frequency	(-500.3, -500.6)
Nucleus	(1H, 1H)
Acquired Size	(1024, 256)
Spectral Size	(1024, 1024)



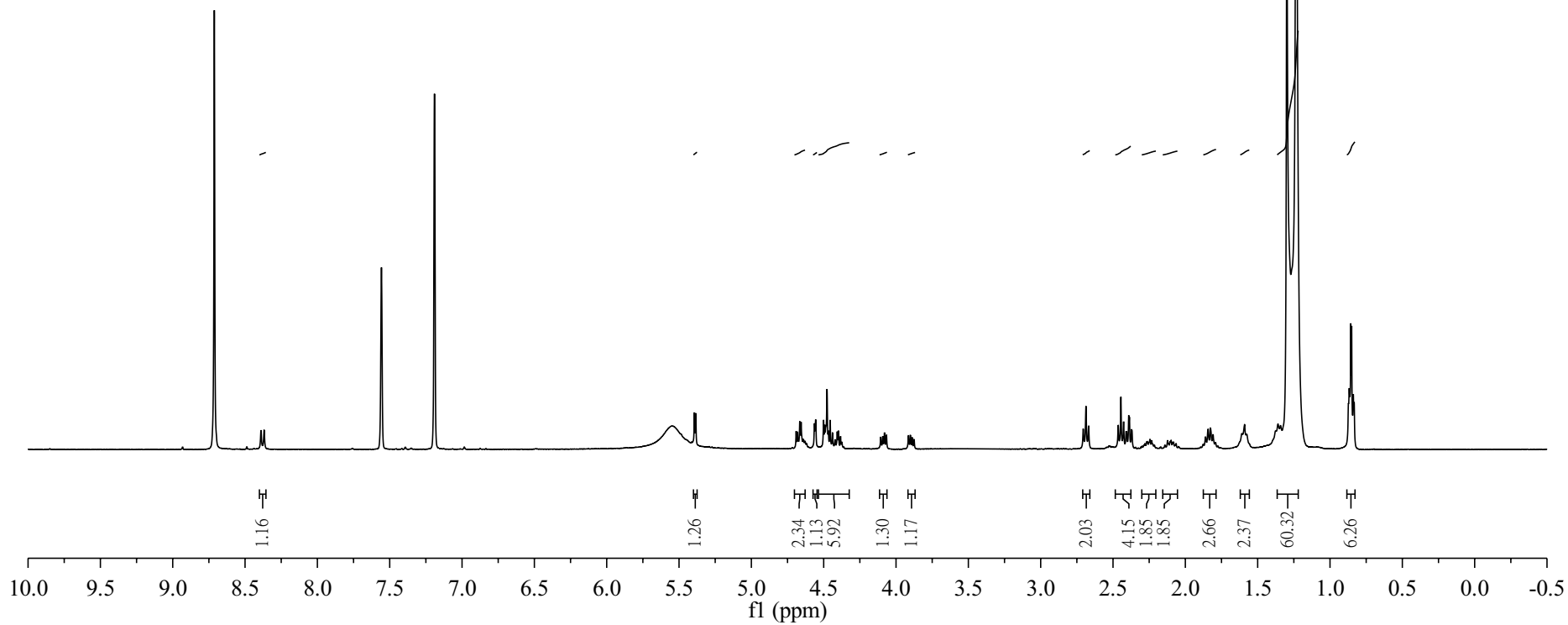
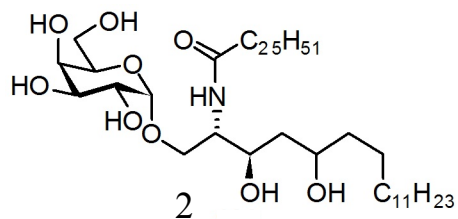


Parameter	Value (f2, f1)
Origin	Varian
Spectrometer	inova
Solvent	CDC13
Temperature	29.0
Pulse Sequence	gHSQC
Experiment	2D-HSQC
Number of Scans	16
Receiver Gain	50
Relaxation Delay	1.0000
Acquisition Time	0.1280
Spectrometer Frequency	(599.94, 150.86)
Spectral Width	(8000.0, 25641.0)
Lowest Frequency	(-504.6, -1545.3)
Nucleus	(1H, 13C)
Acquired Size	(1024, 256)
Spectral Size	(1024, 1024)



Parameter	Value
1 Comment	HSL-262
2 Origin	Varian
3 Spectrometer	nmrs
4 Author	
5 Solvent	pyridine
6 Temperature	25.0
7 Pulse Sequence	s2pul
8 Number of Scans	84
9 Receiver Gain	30
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	2.5559
13 Modification Date	2013-01-03T13:19:24
14 Spectrometer Frequency	399.76
15 Spectral Width	6410.3
16 Lowest Frequency	-927.4
17 Nucleus	<sup>1</sup> H
18 Acquired Size	16384
19 Spectral Size	32768

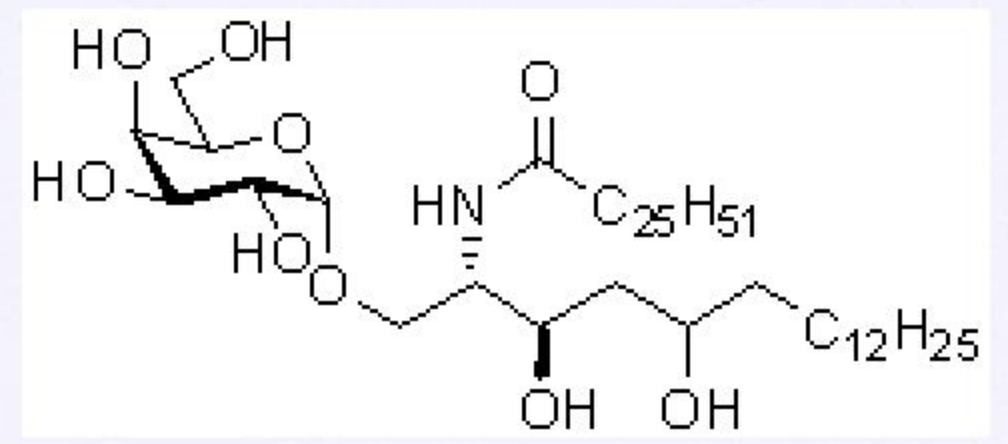
5.546 5.394 5.384 4.690 4.681 4.665 4.656 4.564 4.556 4.501 4.493 4.477 4.468 4.455 4.406 4.397 2.706 2.687 2.669 2.464 2.445 2.445 2.427 2.391 2.387 1.826 1.590 1.360 1.342 1.298 1.237 0.867 0.856 0.850 0.839 0.833



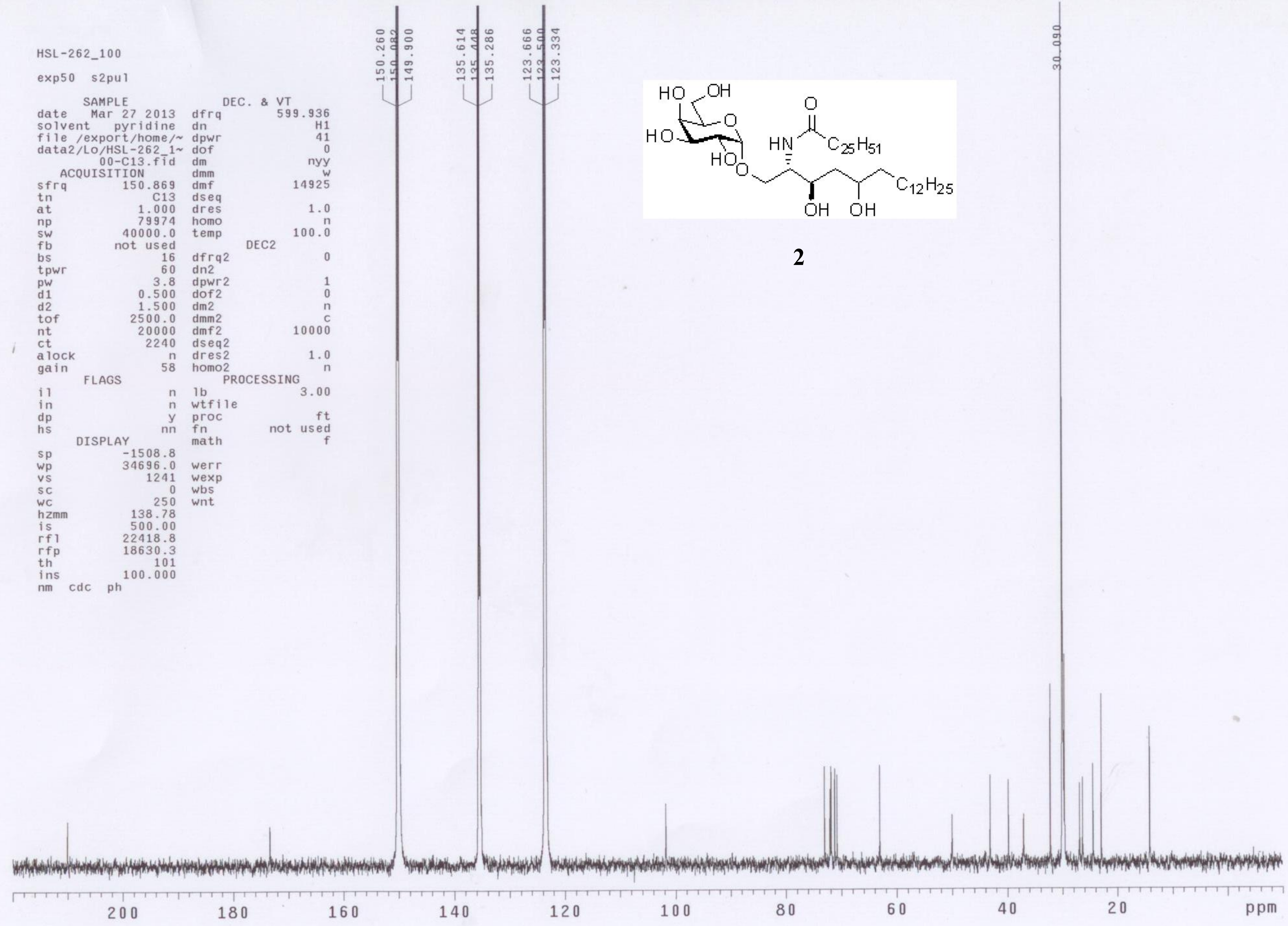
HSL-262\_100

exp50 s2pu1

SAMPLE		DEC. & VT	
date	Mar 27 2013	dfrq	599.936
solvent	pyridine	dn	H1
file	/export/home/~	dpwr	41
data2/Lo/HSL-262_1~		dof	0
00-C13.fid		dm	nyy
ACQUISITION		dmm	w
sfrq	150.869	dmf	14925
tn	C13	dseq	
at	1.000	dres	1.0
np	79974	homo	n
sw	40000.0	temp	100.0
fb	not used	DEC2	
bs	16	dfrq2	0
tpwr	60	dn2	
pw	3.8	dpwr2	1
d1	0.500	dof2	0
d2	1.500	dm2	n
tof	2500.0	dmm2	c
nt	20000	dmf2	10000
ct	2240	dseq2	
alock	n	dres2	1.0
gain	58	homo2	n
FLAGS		PROCESSING	
il	n	lb	3.00
in	n	wtfile	
dp	y	proc	ft
hs	nn	fn	not used
DISPLAY		math	f
sp	-1508.8		
wp	34696.0	werr	
vs	1241	wexp	
sc	0	wbs	
wc	250	wnt	
hzmm	138.78		
is	500.00		
rfl	22418.8		
rfp	18630.3		
th	101		
ins	100.000		
nm	cdc	ph	



2



150.260  
150.082  
149.900

135.614  
135.448  
135.286

123.666  
123.500  
123.334

30.090

200 180 160 140 120 100 80 60 40 20 ppm

HSL-262\_100

Pulse Sequence: DEPT

