

Bifunctional building blocks in Ugi-azide condensation: A general strategy toward lactam-tetrazoles scenarios

Steven Gunawan and Christopher Hulme

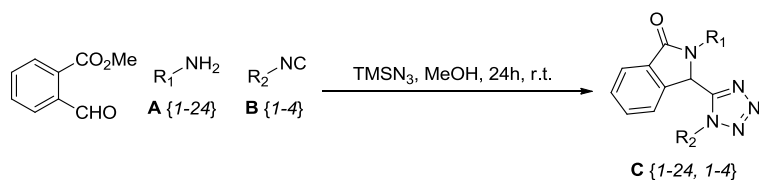
BIO5 Oro Valley, The University of Arizona, 1580 E. Hanley Blvd., Oro Valley, AZ 85737, USA

Table of Contents

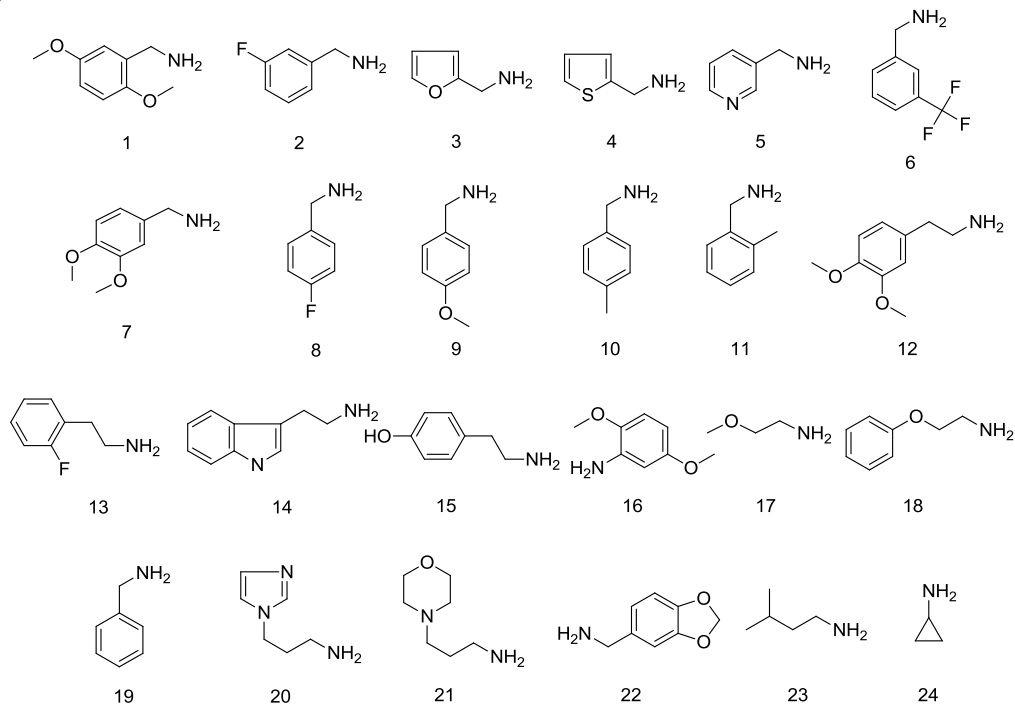
Reagent diversity for the four 24-well plates production of tetrazolyl-indolinones.....	3
General procedure for the syntheses of aldo/keto esters (8b , 19b , 28 , and 30)	4
¹ H NMR of 8b	5
¹³ C NMR of 8b	6
¹ H NMR of 19b	7
¹³ C NMR of 19b	8
¹ H NMR of 28	9
¹³ C NMR of 28	10
¹ H NMR of 30	11
¹³ C NMR of 30	12
¹ H NMR of 10b	13
¹³ C NMR of 10b	14
¹ H NMR of 10c	15
¹³ C NMR of 10c	16
¹ H NMR of 10d	17
¹³ C NMR of 10d	18
¹ H NMR of 10e	19
¹³ C NMR of 10e	20
¹ H NMR of 10f	21
¹³ C NMR of 10f	22
¹ H NMR of 10g	23
¹³ C NMR of 10g	24
¹ H NMR of 10h	25
¹³ C NMR of 10h	26
¹ H NMR of 10i	27
¹³ C NMR of 10i	28
¹ H NMR of 10j	29
¹³ C NMR of 10j	30
¹ H NMR of 20a	31
¹³ C NMR of 20a	32
¹ H NMR of 20b	33
¹³ C NMR of 20b	34
¹ H NMR of 20c	35
¹³ C NMR of 20c	36
¹ H NMR of 20d	37
¹³ C NMR of 20d	38
¹ H NMR of 20e	39
¹³ C NMR of 20e	40
¹ H NMR of 22a	41
¹³ C NMR of 22a	42
¹ H NMR of 22b	43
¹³ C NMR of 22b	44
¹ H NMR of 22c	45
¹³ C NMR of 22c	46
¹ H NMR of 22d	47
¹³ C NMR of 22d	48
¹ H NMR of 22e	49
¹³ C NMR of 22e	50
¹ H NMR of 22f	51
¹³ C NMR of 22f	52

¹ H NMR of 24a	53
¹³ C NMR of 24a	54
¹ H NMR of 24b	55
¹³ C NMR of 24b	56
¹ H NMR of 24c	57
¹³ C NMR of 24c	58
¹ H NMR of 24d	59
¹³ C NMR of 24d	60
¹ H NMR of 24e	61
¹³ C NMR of 24e	62
¹ H NMR of 29a	63
¹³ C NMR of 29a	64
¹ H NMR of 29b	65
¹³ C NMR of 29b	66
¹ H NMR of 29c	67
¹³ C NMR of 29c	68
¹ H NMR of 29d	69
¹³ C NMR of 29d	70
¹ H NMR of 29e	71
¹³ C NMR of 29e	72
¹ H NMR of 31a	73
¹³ C NMR of 31a	74
¹ H NMR of 31b	75
¹³ C NMR of 31b	76
¹ H NMR of 31c	77
¹³ C NMR of 31c	78
¹ H NMR of 31d	79
¹³ C NMR of 31d	80
¹ H NMR of 31e	81
¹³ C NMR of 31e	82
¹ H NMR of 31f	83
¹³ C NMR of 31f	84

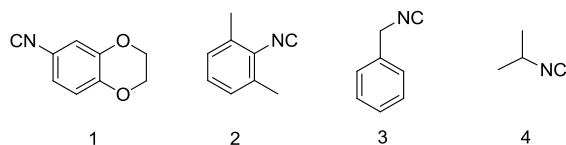
Reagents diversity for the four 24-well plate production of tetrazolyl-indolinones **10**



Primary amines (**A**)



Isocyanides (**B**)



Yield and purity (%) of the 96-well plate production of **C** {1-24, 1-4}

R₁NH₂ (A)	R₂NC (B)								R₁NH₂ (A)	R₂NC (B)							
	1		2		3		4			1		2		3		4	
	Y	P	Y	P	Y	P	Y	P		Y	P	Y	P	Y	P	Y	P
1	29	100	3	100	31	100	34	100	13	22	100	9	100	23	98	18	100
2	27	100	nr	-	21	100	27	100	14	34	100	nr	-	30	100	30	100
3	26	100	nr	-	21	100	8	100	15	20	100	26	100	21	100	34	99*
4	36	100	2	100	31	100	8	91	16	6	100	4	100*	nr	-	nr	-
5	38	100	nr	-	8	100	8	100	17	22	100	5	100	16	100	17	100
6	32	100	1	100	24	100	5	100	18	44	100	28	100	26	98	34	100
7	32	100	22	100	22	100	34	95	19	39	98	84	100	4	100	33	100
8	24	100	nr	-	28	100	34	100	20	39	100	42	100*	27	100	39	100
9	24	100	nr	-	14	98	25	100	21	15	100	11	100	24	100	32	100
10	33	100	30	100*	nr	-	19	100	22	26	100	1	100	13	100	5	100
11	31	100	nr	-	7	100	30	100	23	16	100	24	96	28	100	28	100
12	26	100	44	100	26	100	31	100	24	25	100	32	100	25	93	27	100

Y = Yield (%); P = Purity (%) based on UV 214 nm; nr = not recovered/lost during purification; * purity based on ELS

General experimental procedure for synthesis of methyl 2-formylbenzoate (8b)

To a stirred 2-carboxybenzaldehyde (2.108 g, 14.04 mmol) in MeOH (3.00 ml)-hexanes (38.00 ml) was added 2M TMSCHN₂ in hexanes (12.00 ml) via syringe dropwise at room temperature. The mixture was stirred for 2 h and upon completion was concentrated *in vacuo* to afford the methyl 2-formylbenzoate **3c** (2.108 g, 12.84 mmol, 91%) as a clear oil. [M+H]⁺ = 165. ¹H NMR (400 MHz, CDCl₃) δ ppm 10.62 (s, 1H), 8.01 – 7.91 (m, 2H), 7.69 – 7.61 (m, 2H), 3.98 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ ppm 192.0, 166.7, 137.0, 132.9, 132.4, 131.9, 130.3, 128.4, 52.7.

General experimental procedure for synthesis of methyl 2-((2-oxopropyl)thio)acetate (19b)

Methyl 2-mercaptoacetate (1.967 ml, 22.00 mmol) and triethylamine (5.58 ml, 40.00 mmol) were stirred in anhydrous DCM (50 ml) at 0 °C. Chloroacetone (1.609 ml, 20.00 mmol) was added and the reaction was stirred for 4h. Upon completion, the mixture was diluted in EtOAc (50ml), washed with saturated NaHCO₃ solution (2 x 75 ml) and brine solution (75 ml). The organic layer was dried over Na₂SO₄ and concentrated *in vacuo* to afford methyl 2-((2-oxopropyl)thio)acetate **17b** (2.90 g, 17.88 mmol, 89%) as a yellow oil. [M+H]⁺ = 163. ¹H NMR (400 MHz, CDCl₃) δ ppm 3.73 (s, 3H), 3.42 (s, 2H), 3.27 (s, 2H), 2.29 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ ppm 202.8, 170.1, 52.4, 42.1, 33.1, 28.2.

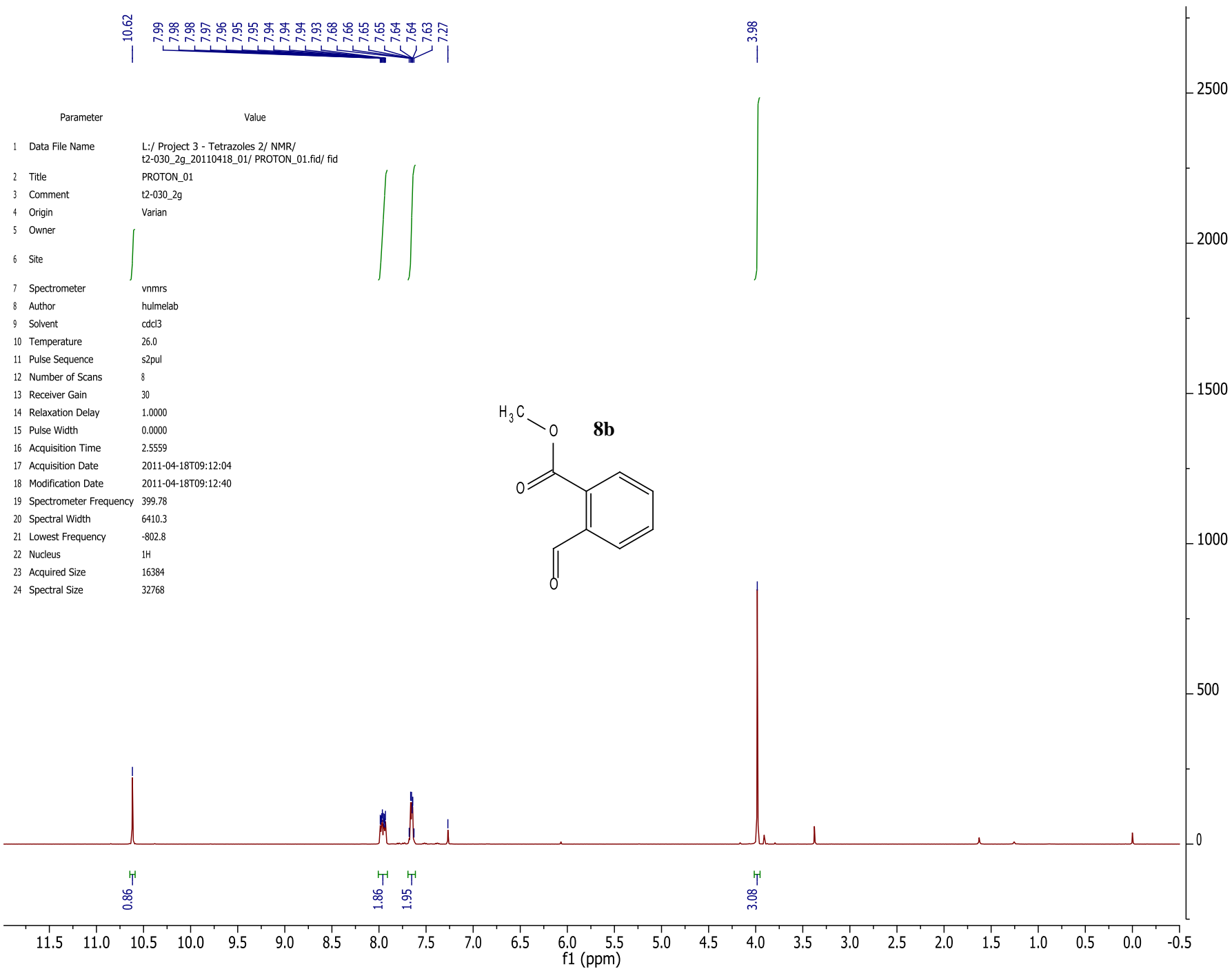
General experimental procedure for synthesis of methyl 2-((3-oxobutyl)thio)acetate (28)

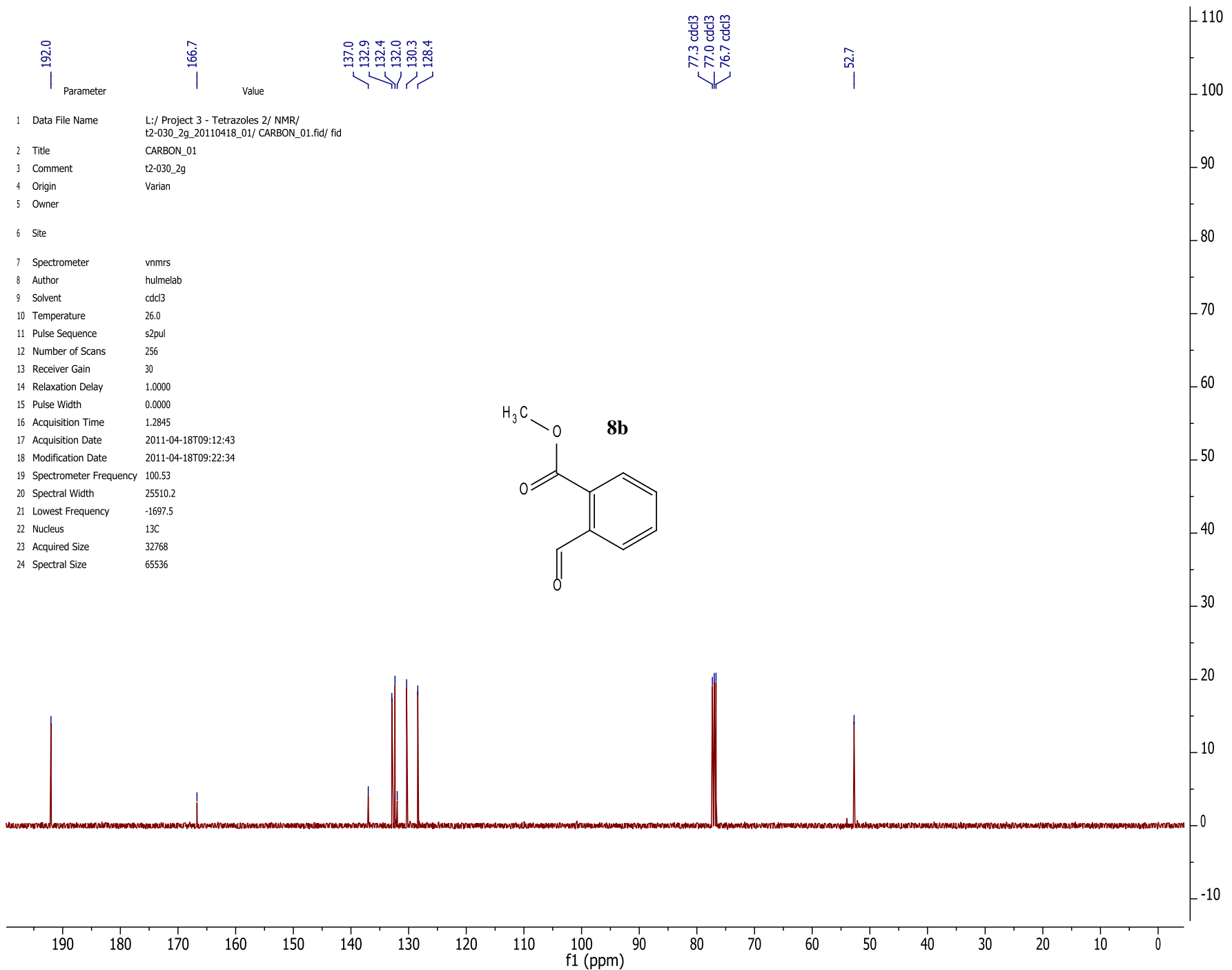
Methyl 2-mercaptoacetate (1.967 ml, 22.00 mmol) and triethylamine (5.58 ml, 40.00 mmol) were stirred in anhydrous DCM (20 ml) at 0 °C. 4-chlorobutan-2-one (2.131 g, 20.00 mmol) dissolved in DCM (40 ml) was then added dropwise and the reaction was stirred for 4h. Upon completion, the mixture was diluted in EtOAc (50ml), washed with saturated NaHCO₃ solution (2 x 75 ml) and brine solution (75 ml). The organic layer was dried over Na₂SO₄ and concentrated *in vacuo* to afford methyl 2-((3-oxobutyl)thio)acetate **26** (1.95 g, 11.06 mmol, 55%) of a yellow oil. [M+H]⁺ = 177. ¹H NMR (400 MHz, CDCl₃) δ ppm 3.74 (s, 3H), 3.26 (s, 2H), 2.87 (t, *J* = 7.1 Hz, 2H), 2.78 (t, *J* = 6.9 Hz, 2H), 2.18 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ ppm 206.34, 170.80, 77.32, 77.00, 76.69, 52.41, 43.14, 33.84, 29.98, 26.43.

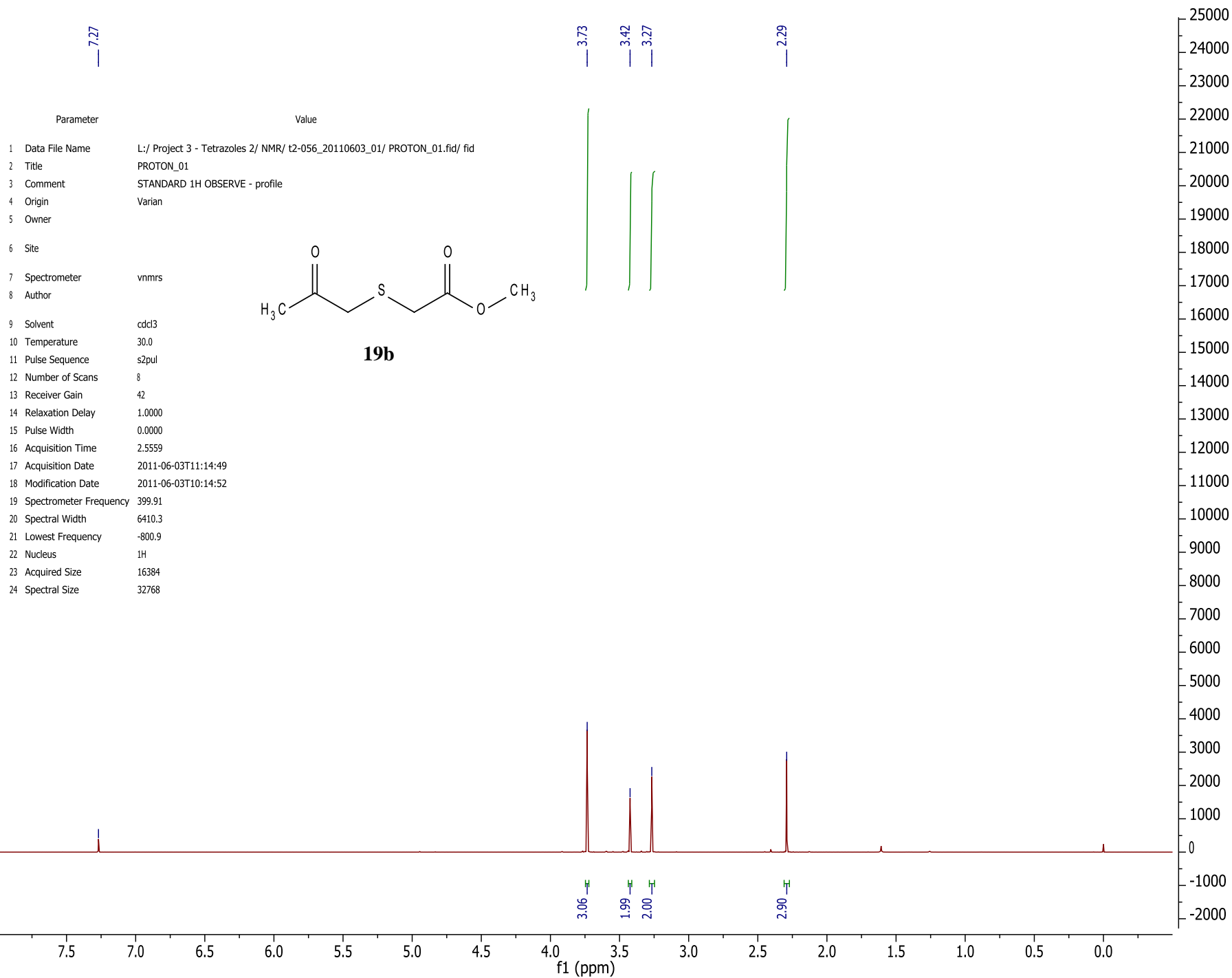
General experimental procedure for synthesis of methyl 2-(2-formylphenoxy)acetate (30)

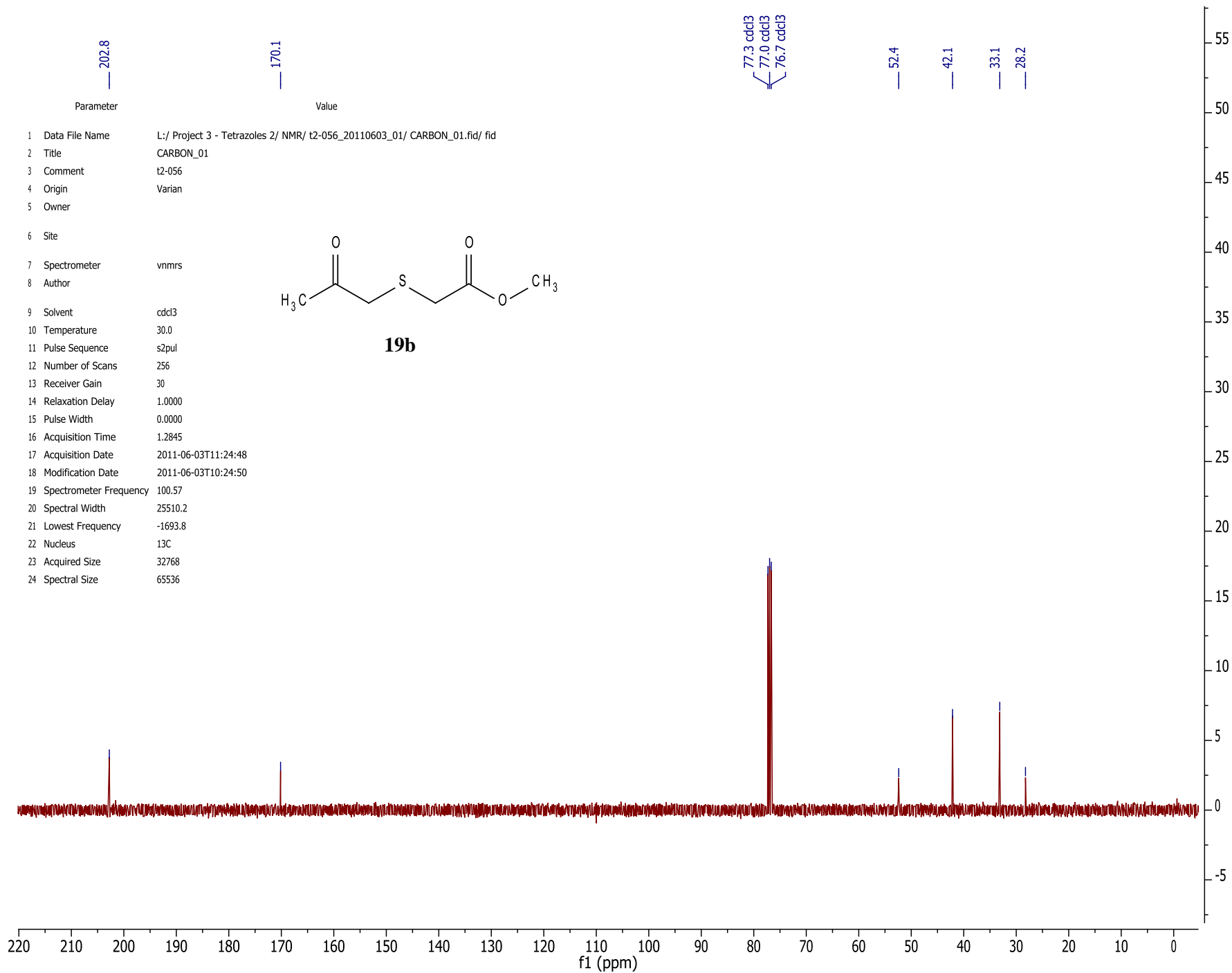
A stirred 2-(2-formylphenoxy)acetic acid (6.000 g, 33.3 mmol) in MeOH (40 ml) was treated with a 37% solution of hydrochloric acid (5.06 ml) and refluxed for 12 hours. The solution was cooled to room temperature and concentrated *in vacuo*. EtOAc was added and the organic layer was washed with 5% aqueous solution of NaHCO₃ followed by brine, dried over MgSO₄ and concentrated *in vacuo* to afford methyl 2-(2-formylphenoxy)acetate **28** (5.89 g, 30.3 mmol, 91%) of a light brown solid. [M+H]⁺ = 195. ¹H NMR (400 MHz, CDCl₃) δ ppm 10.57 (s, 1H), 7.87 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.58 – 7.50 (m, 1H), 7.10 (td, *J* = 7.6, 0.5 Hz, 1H), 6.86 (d, *J* = 8.4 Hz, 1H), 4.78 (s, 2H), 3.82 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ ppm 189.5, 168.6, 160.0, 135.7, 128.7, 125.4, 121.9, 112.5, 65.5, 52.4.

Note: **8b**, **19b**, **28**, and **30** were used immediately in the Ugi-azide MCR without purification

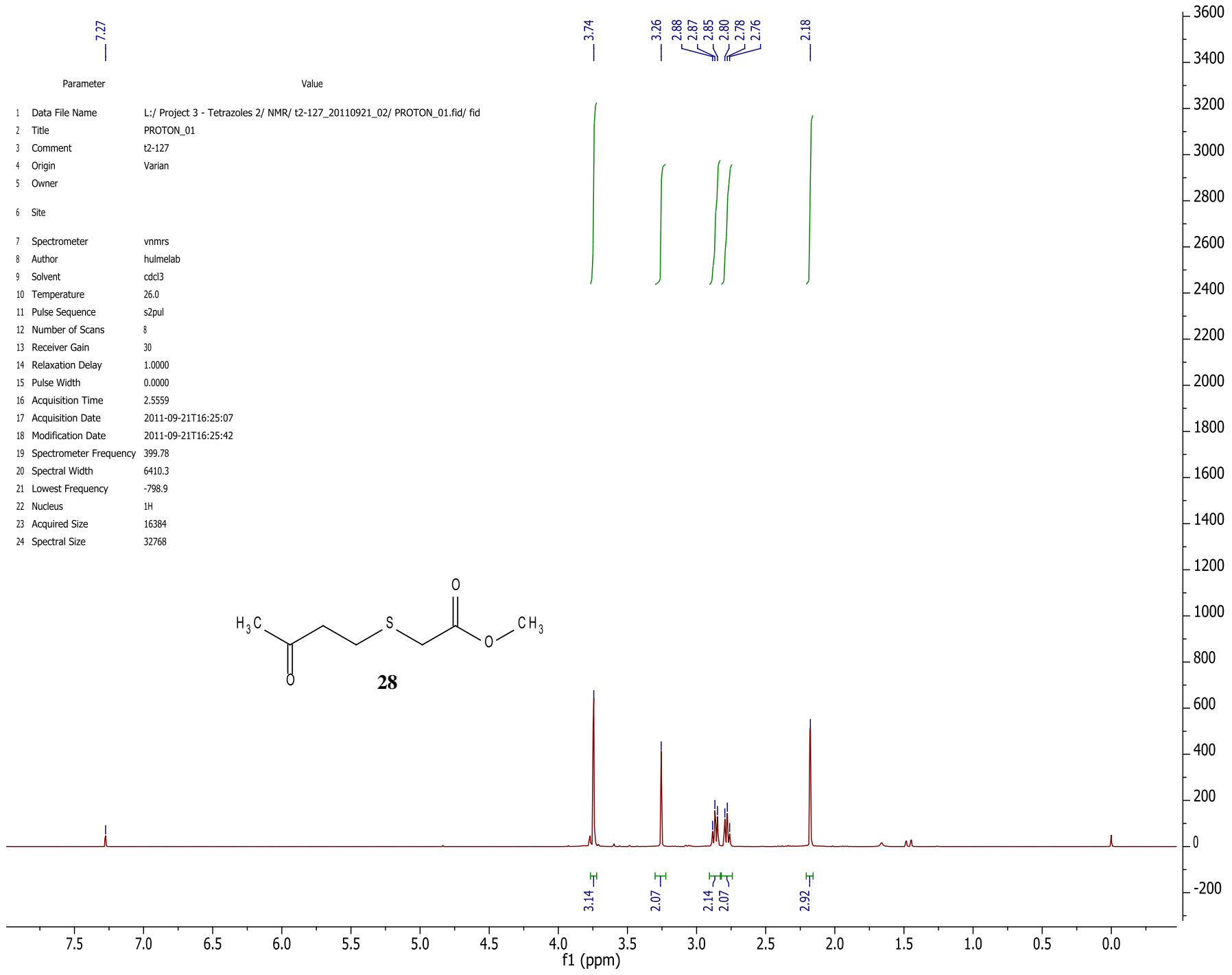
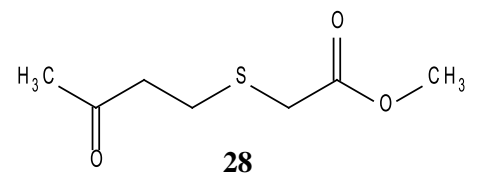


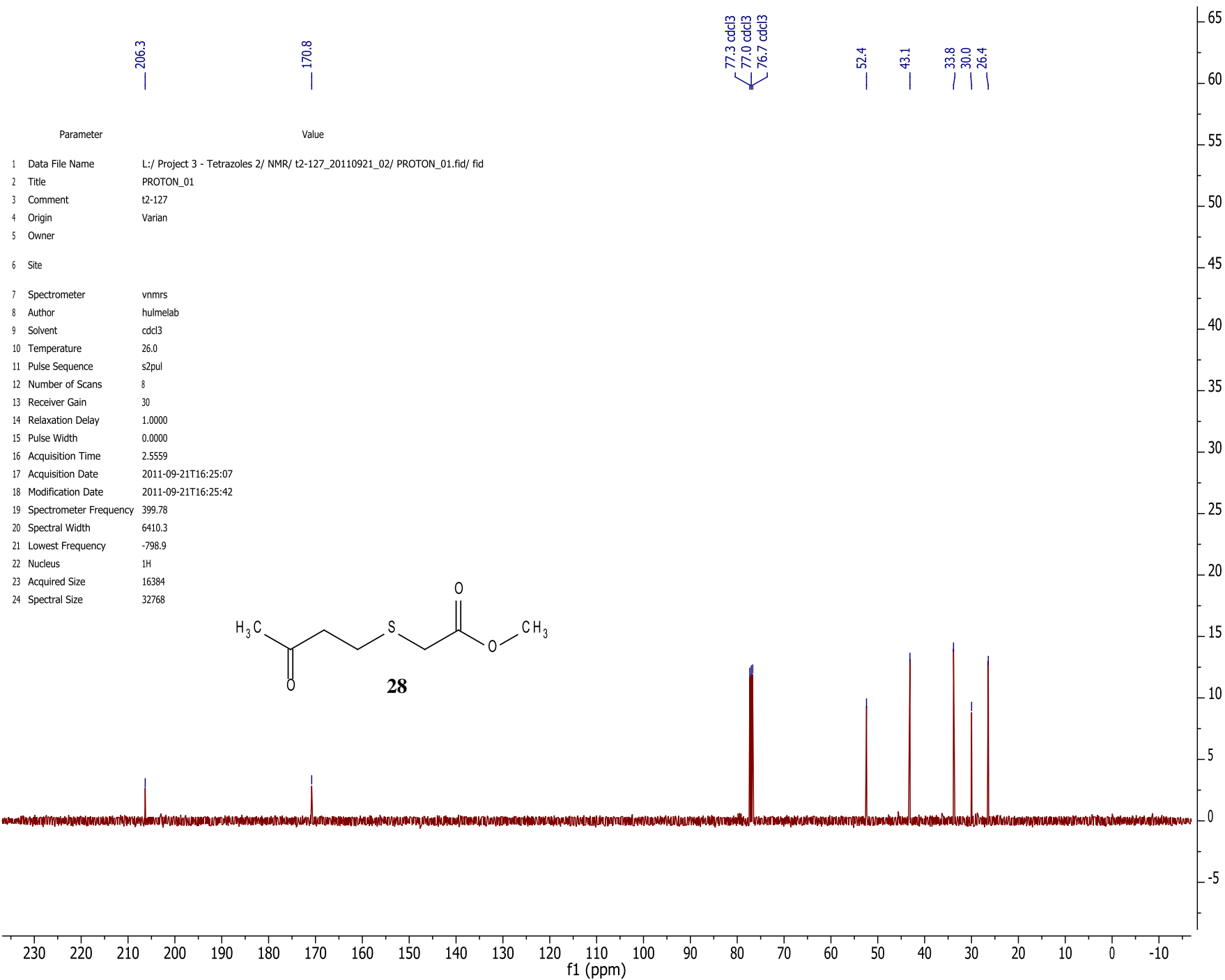




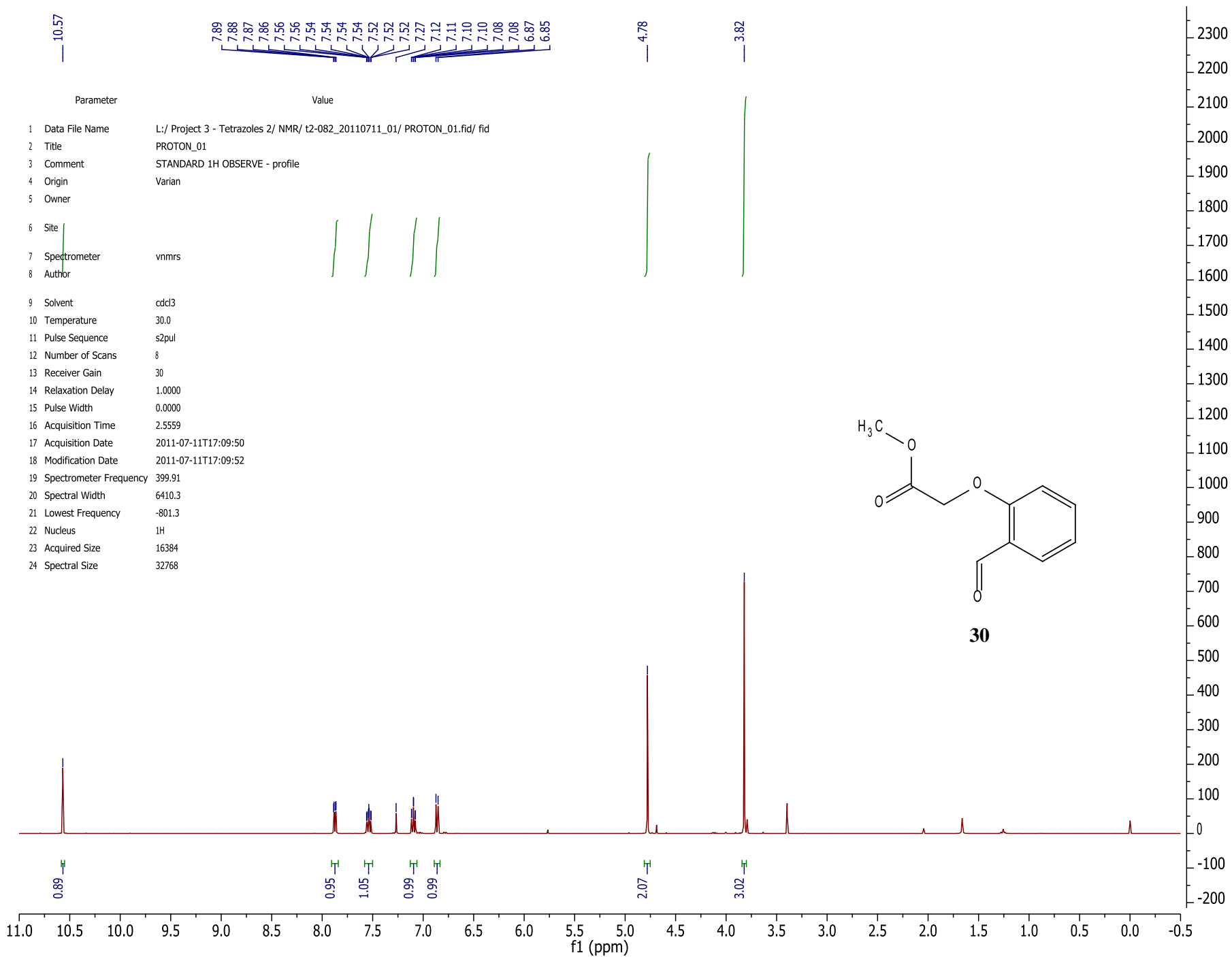


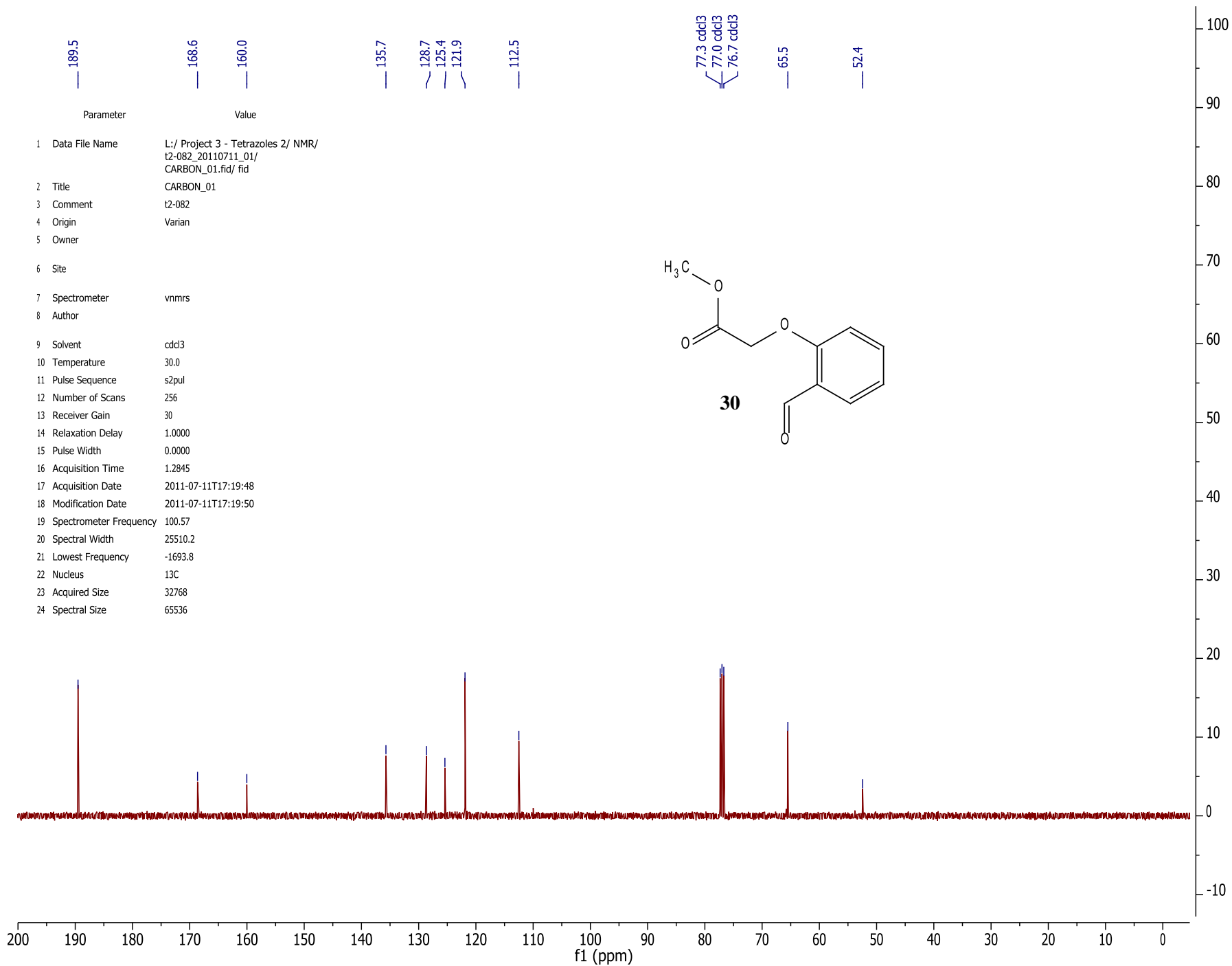
Parameter	Value
1 Data File Name	L:/ Project 3 - Tetrazoles 2/ NMR/ t2-127_20110921_02/ PROTON_01.fid/ fid
2 Title	PROTON_01
3 Comment	t2-127
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	nmrs
8 Author	hulmelab
9 Solvent	cdcl3
10 Temperature	26.0
11 Pulse Sequence	s2pul
12 Number of Scans	8
13 Receiver Gain	30
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	2.5559
17 Acquisition Date	2011-09-21T16:25:07
18 Modification Date	2011-09-21T16:25:42
19 Spectrometer Frequency	399.78
20 Spectral Width	6410.3
21 Lowest Frequency	-798.9
22 Nucleus	¹ H
23 Acquired Size	16384
24 Spectral Size	32768

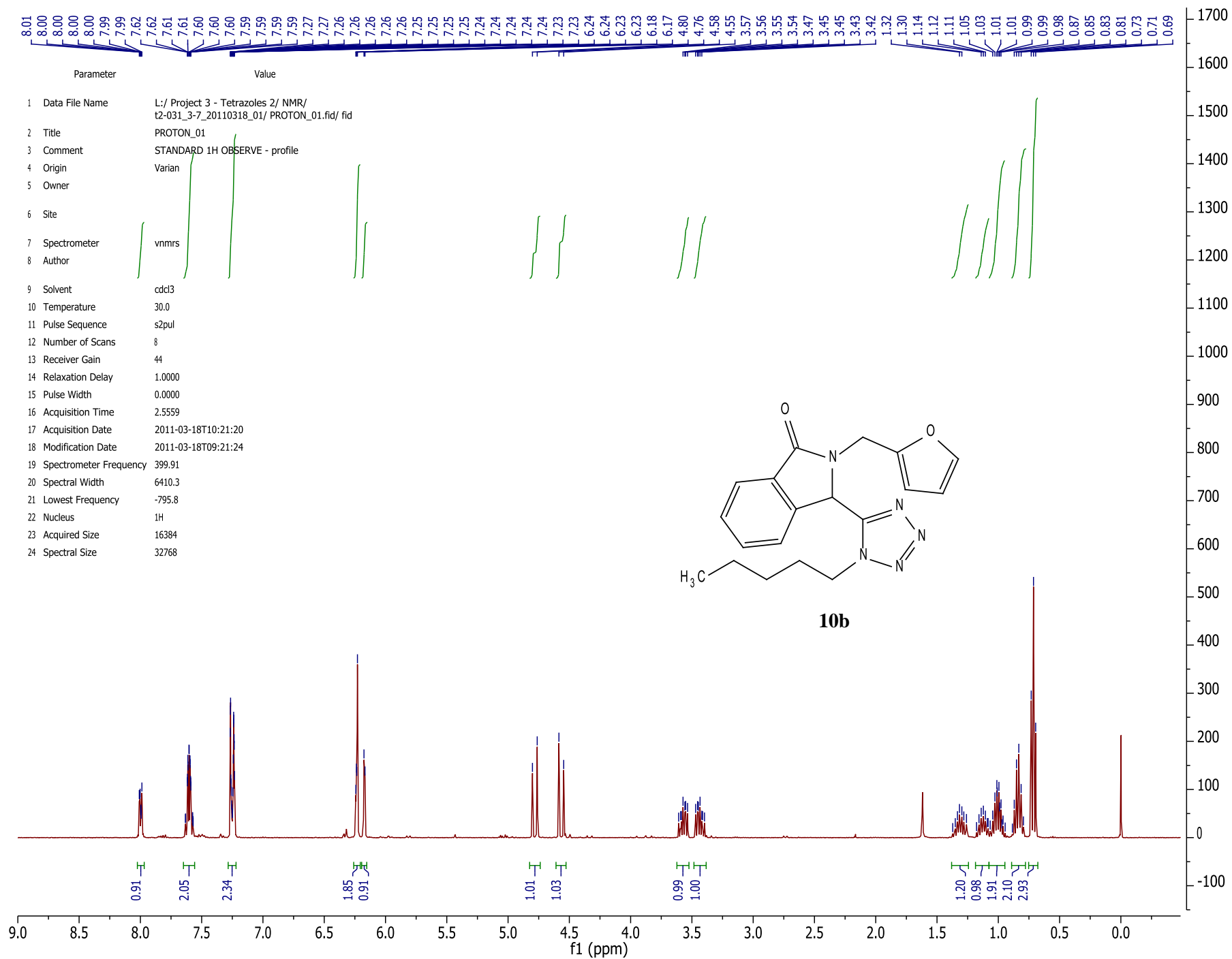


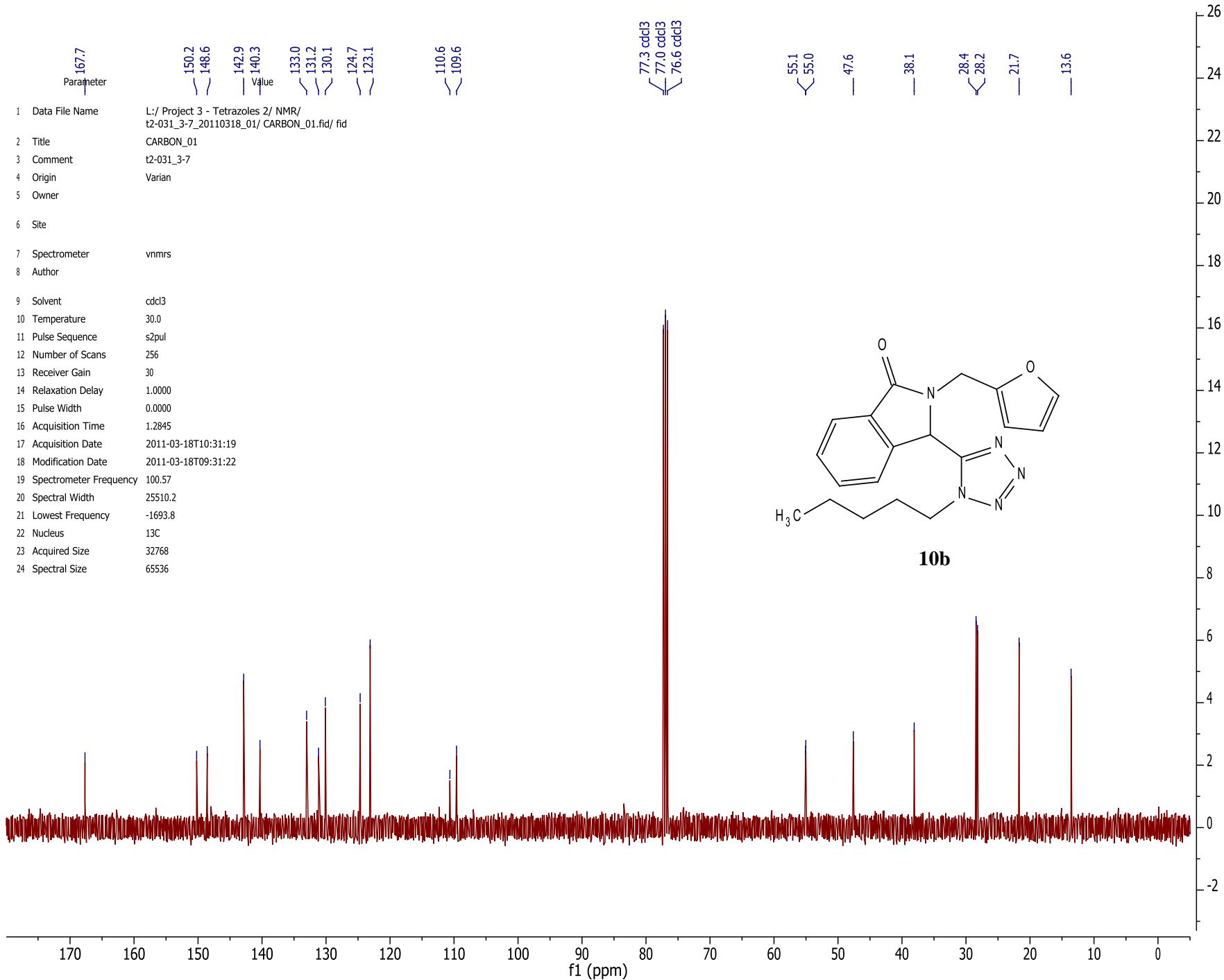


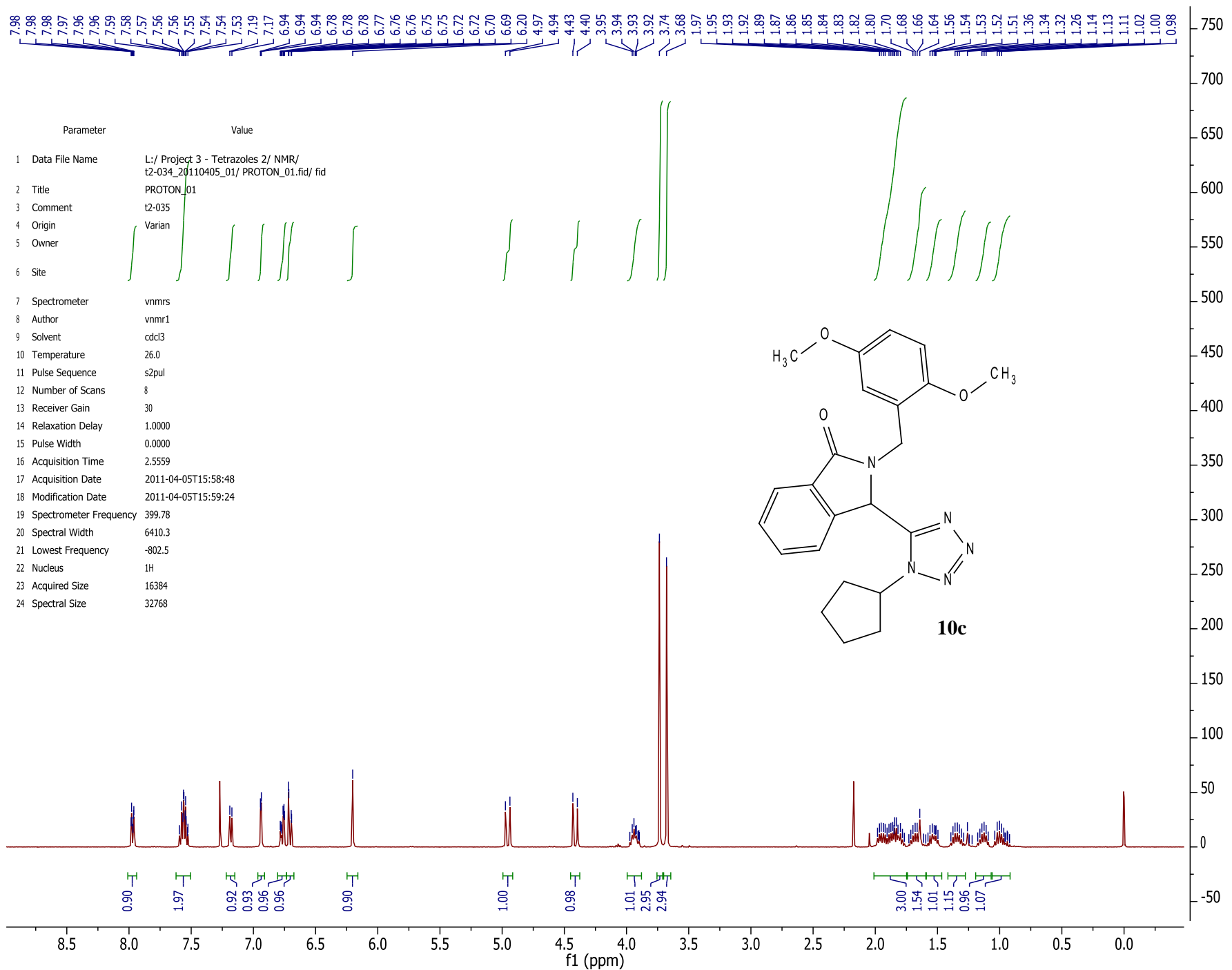
Parameter	Value
1 Data File Name	L:/ Project 3 - Tetrazoles 2/ NMR/ t2-127_20110921_02/ PROTON_01.fid/ fid
2 Title	PROTON_01
3 Comment	t2-127
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	hulmelab
9 Solvent	cdcl3
10 Temperature	26.0
11 Pulse Sequence	s2pul
12 Number of Scans	8
13 Receiver Gain	30
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	2.5559
17 Acquisition Date	2011-09-21T16:25:07
18 Modification Date	2011-09-21T16:25:42
19 Spectrometer Frequency	399.78
20 Spectral Width	6410.3
21 Lowest Frequency	-798.9
22 Nucleus	1H
23 Acquired Size	16384
24 Spectral Size	32768





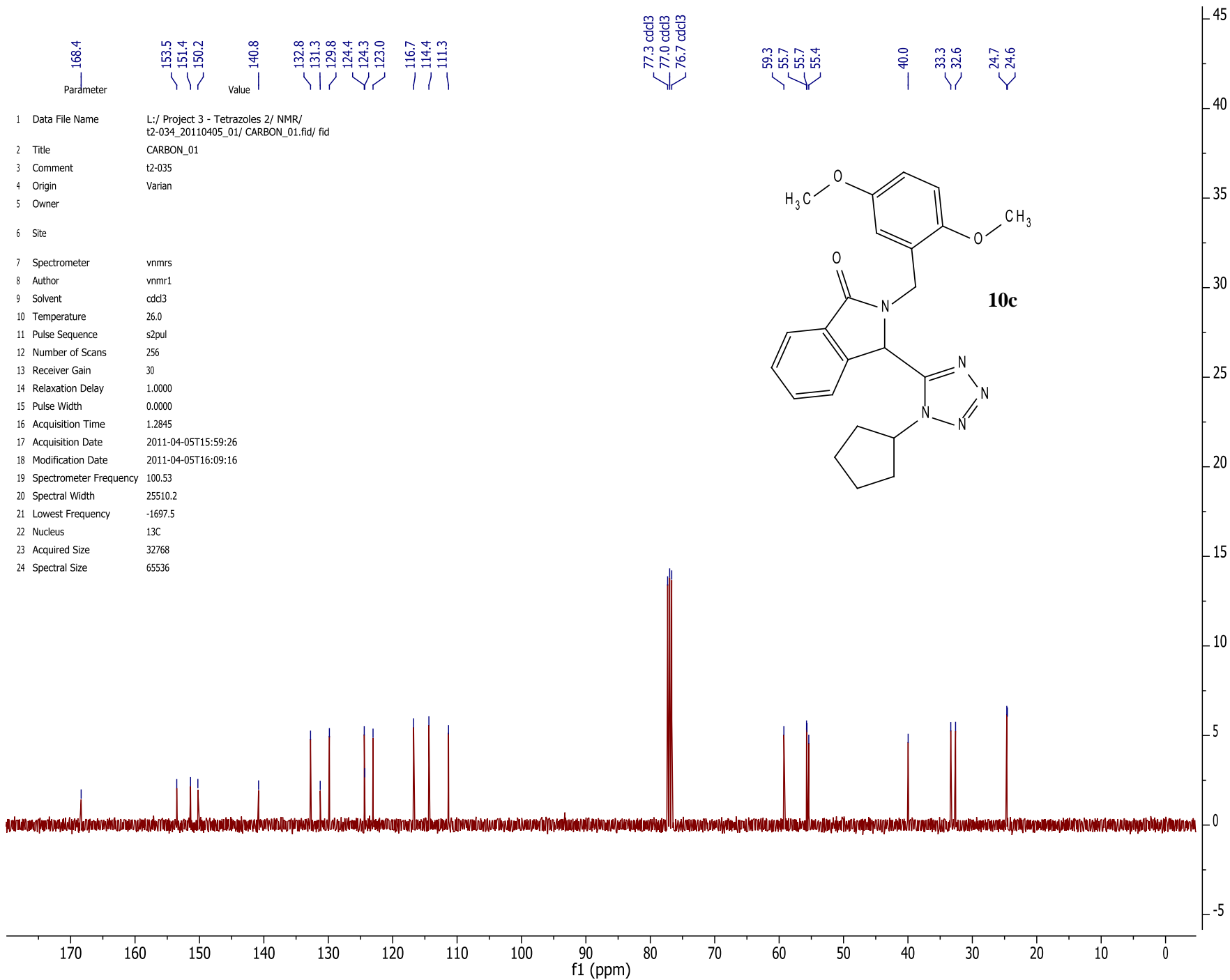


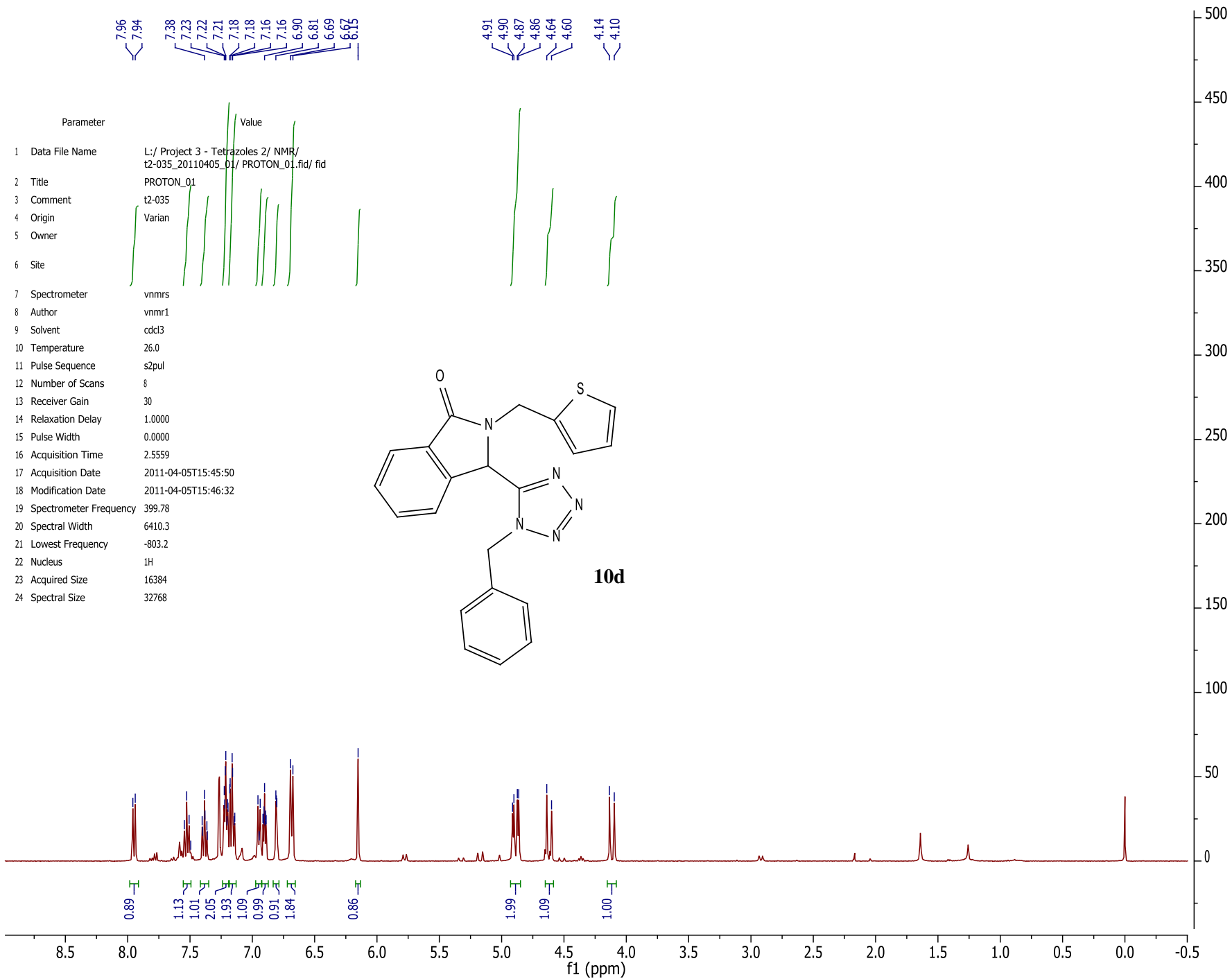


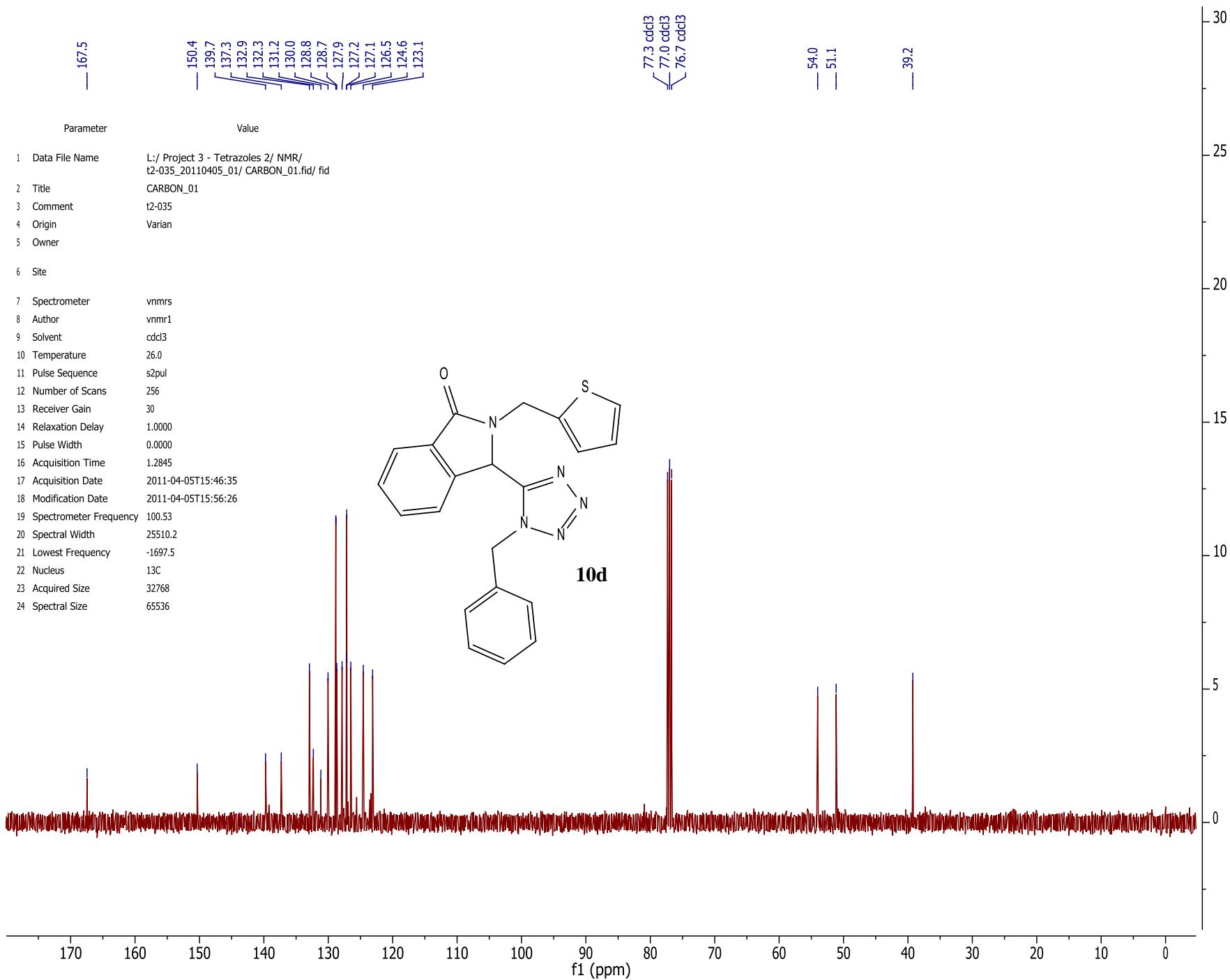


7.98
7.98
7.97
7.96
7.96
7.59
7.58
7.57
7.56
7.55
7.54
7.54
7.53
7.19
7.17
6.94
6.94
6.94
6.78
6.78
6.77
6.76
6.75
6.75
6.75
6.72
6.72
6.70
6.69
6.20
4.97
4.94
4.43
4.40
3.95
3.94
3.93
3.92
3.74
3.68
1.97
1.95
1.93
1.92
1.89
1.87
1.86
1.85
1.84
1.83
1.82
1.80
1.70
1.68
1.66
1.64
1.56
1.54
1.53
1.52
1.51
1.36
1.34
1.32
1.26
1.14
1.13
1.11
1.02
1.00
0.98

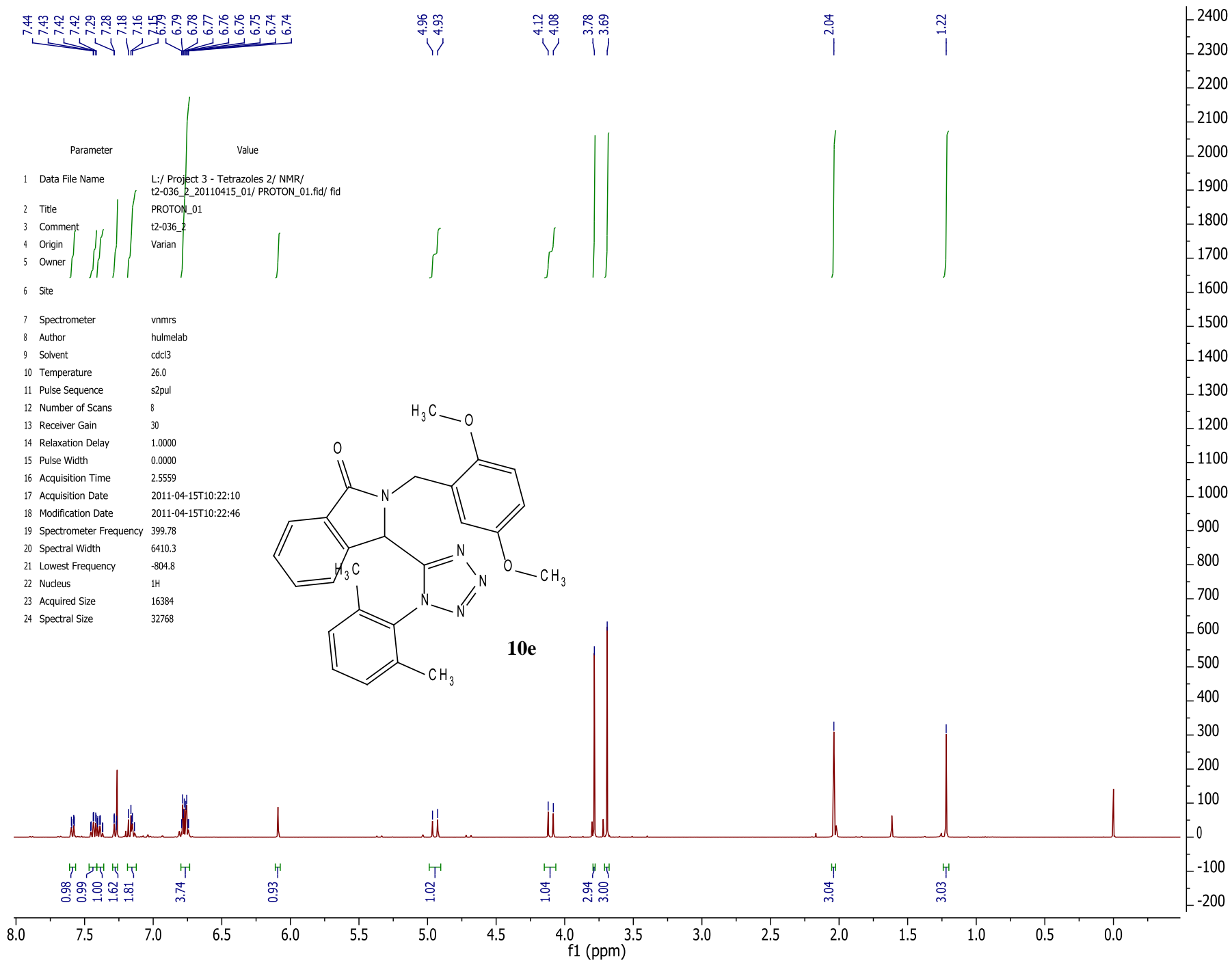
Parameter	Value
1 Data File Name	L:/ Project 3 - Tetrazoles 2/ NMR/ t2-034_20110405_01/ PROTON_01.fid/ fid
2 Title	PROTON_01
3 Comment	t2-035
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	vnmr1
9 Solvent	cdcl3
10 Temperature	26.0
11 Pulse Sequence	s2pul
12 Number of Scans	8
13 Receiver Gain	30
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	2.5559
17 Acquisition Date	2011-04-05T15:58:48
18 Modification Date	2011-04-05T15:59:24
19 Spectrometer Frequency	399.78
20 Spectral Width	6410.3
21 Lowest Frequency	-802.5
22 Nucleus	1H
23 Acquired Size	16384
24 Spectral Size	32768



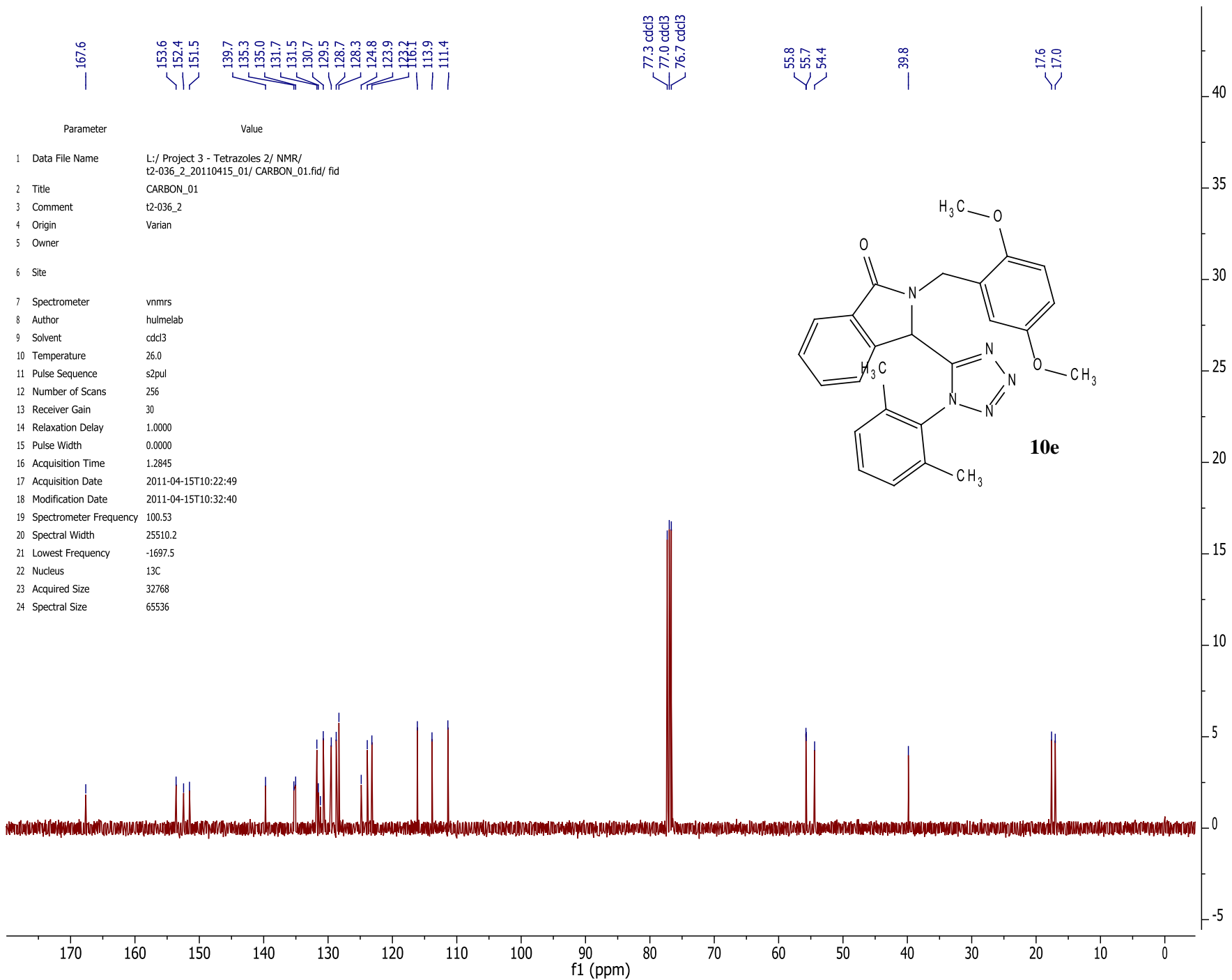
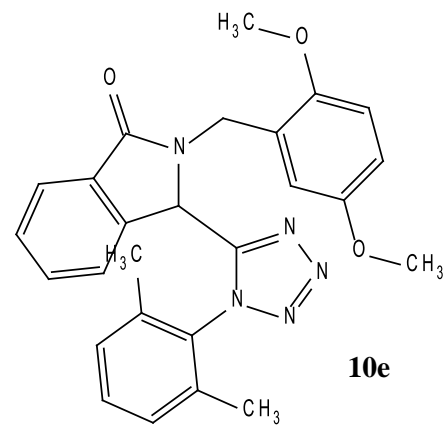




Parameter	Value
1 Data File Name	L:/ Project 3 - Tetrazoles 2/ NMR/ t2-035_20110405_01/ CARBON_01.fid/ fid
2 Title	CARBON_01
3 Comment	t2-035
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnms
8 Author	vnmr1
9 Solvent	cdcl3
10 Temperature	26.0
11 Pulse Sequence	s2pul
12 Number of Scans	256
13 Receiver Gain	30
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.2845
17 Acquisition Date	2011-04-05T15:46:35
18 Modification Date	2011-04-05T15:56:26
19 Spectrometer Frequency	100.53
20 Spectral Width	25510.2
21 Lowest Frequency	-1697.5
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536



Parameter	Value
1 Data File Name	L:/ Project 3 - Tetrazoles 2/ NMR/ t2-036_2_20110415_01/ PROTON_01.fid/ fid
2 Title	PROTON_01
3 Comment	t2-036_2
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	hulmelab
9 Solvent	cdcl3
10 Temperature	26.0
11 Pulse Sequence	s2pul
12 Number of Scans	8
13 Receiver Gain	30
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	2.5559
17 Acquisition Date	2011-04-15T10:22:10
18 Modification Date	2011-04-15T10:22:46
19 Spectrometer Frequency	399.78
20 Spectral Width	6410.3
21 Lowest Frequency	-804.8
22 Nucleus	1H
23 Acquired Size	16384
24 Spectral Size	32768

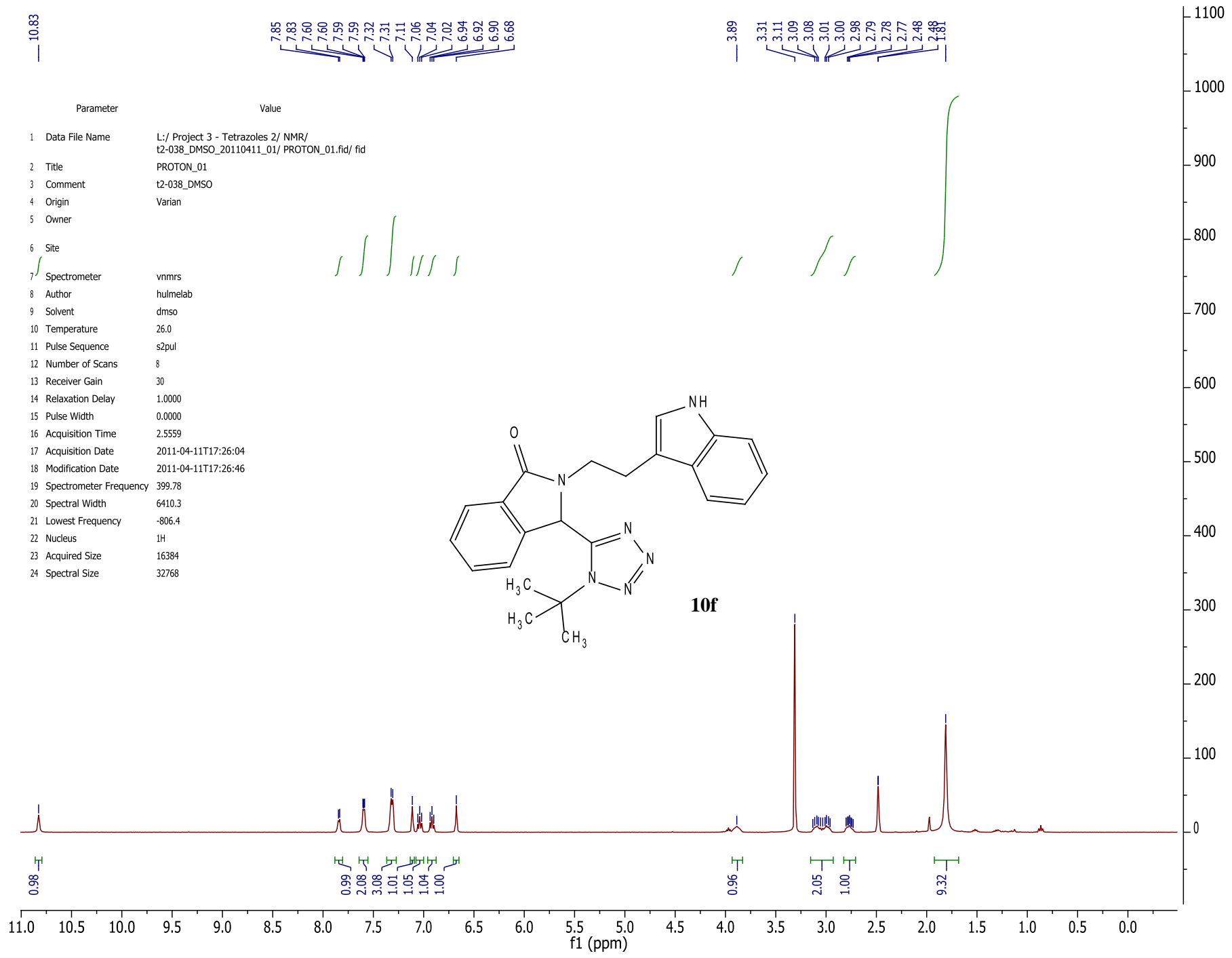
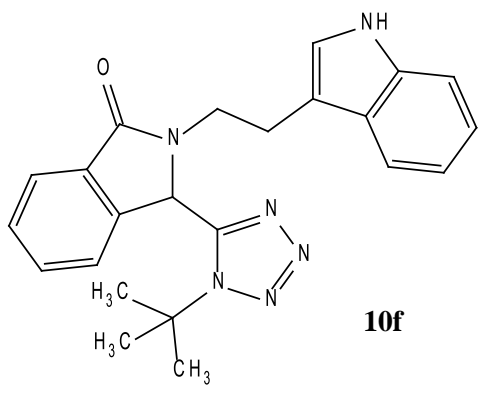


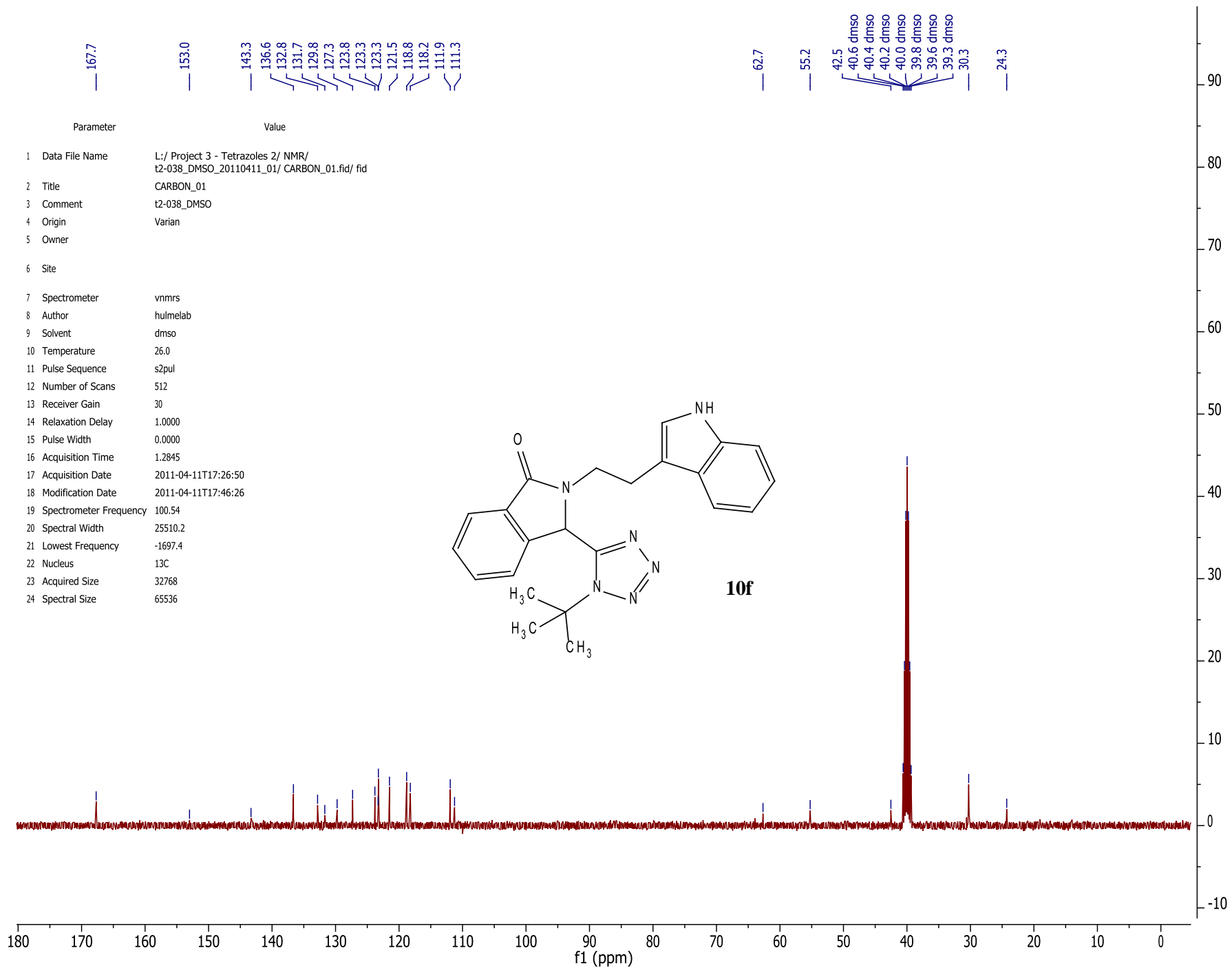
10.83

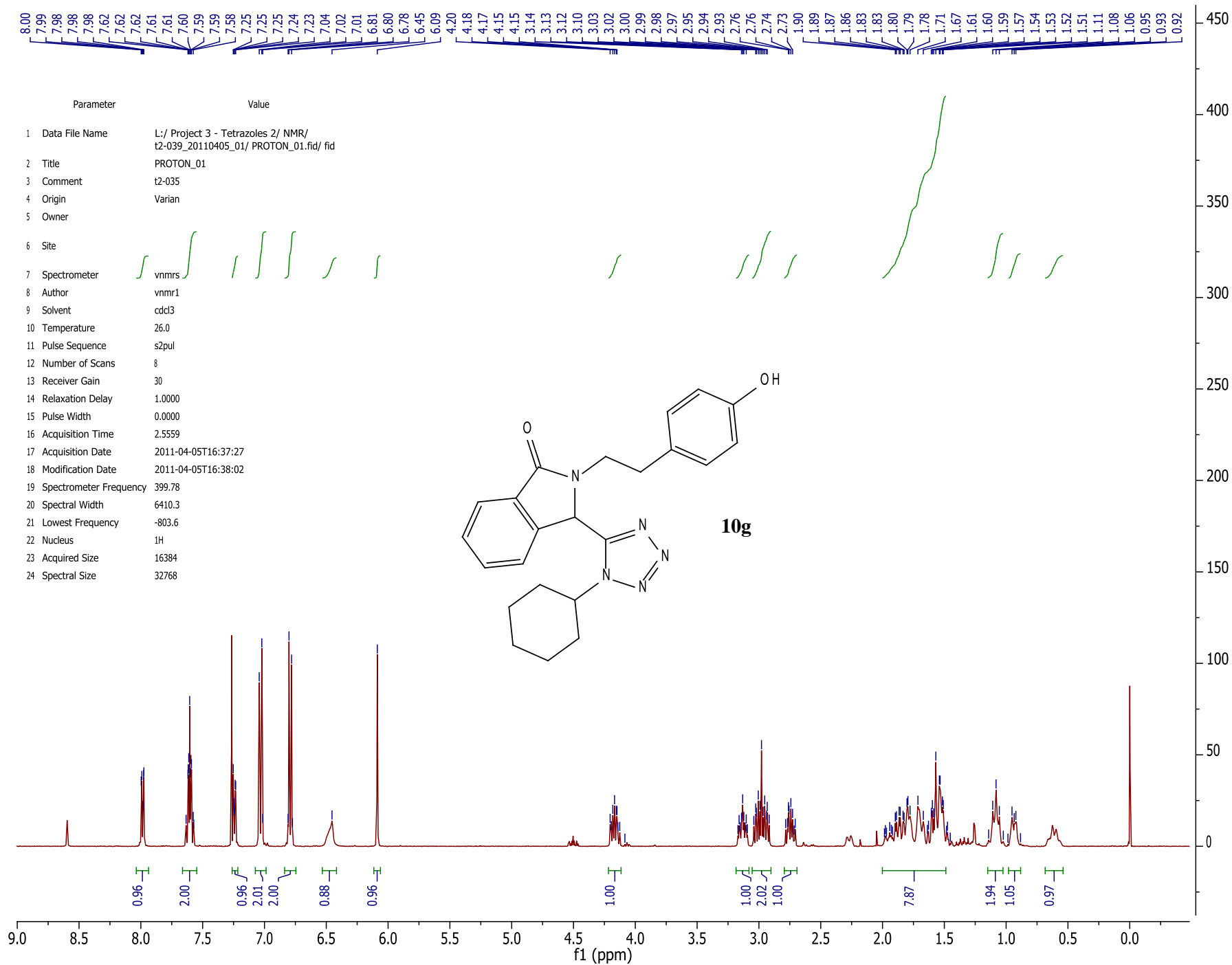
7.85
7.83
7.60
7.60
7.59
7.59
7.32
7.31
7.11
7.06
7.04
7.02
6.94
6.90
6.68

3.89
3.31
3.11
3.09
3.08
3.01
3.00
2.98
2.79
2.78
2.77
2.48
2.48
1.81

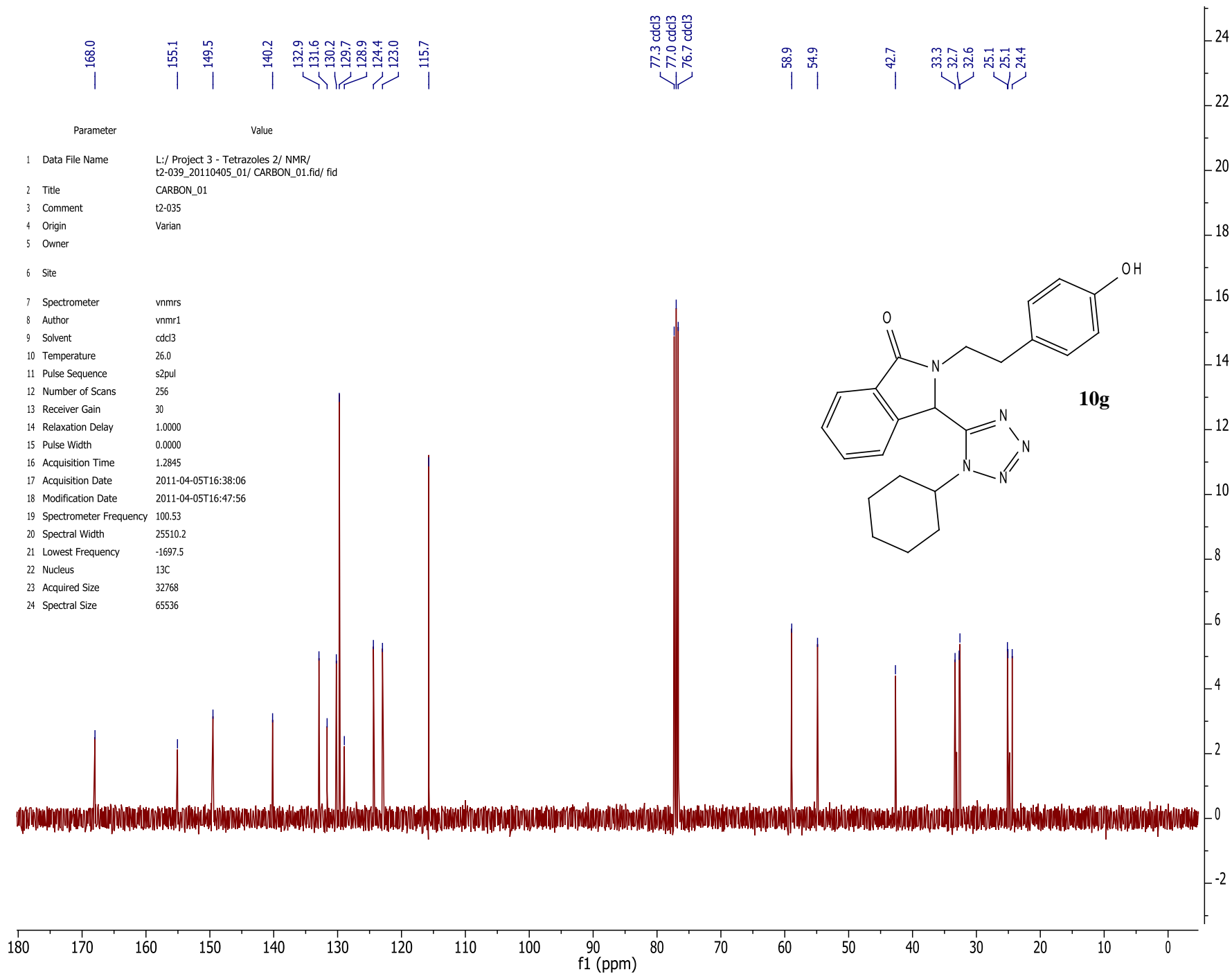
Parameter	Value
1 Data File Name	L:/ Project 3 - Tetrazoles 2/ NMR/ t2-038_DMSO_20110411_01/ PROTON_01.fid/ fid
2 Title	PROTON_01
3 Comment	t2-038_DMSO
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	nmr
8 Author	hulmelab
9 Solvent	dms
10 Temperature	26.0
11 Pulse Sequence	s2pul
12 Number of Scans	8
13 Receiver Gain	30
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	2.5559
17 Acquisition Date	2011-04-11T17:26:04
18 Modification Date	2011-04-11T17:26:46
19 Spectrometer Frequency	399.78
20 Spectral Width	6410.3
21 Lowest Frequency	-806.4
22 Nucleus	¹ H
23 Acquired Size	16384
24 Spectral Size	32768

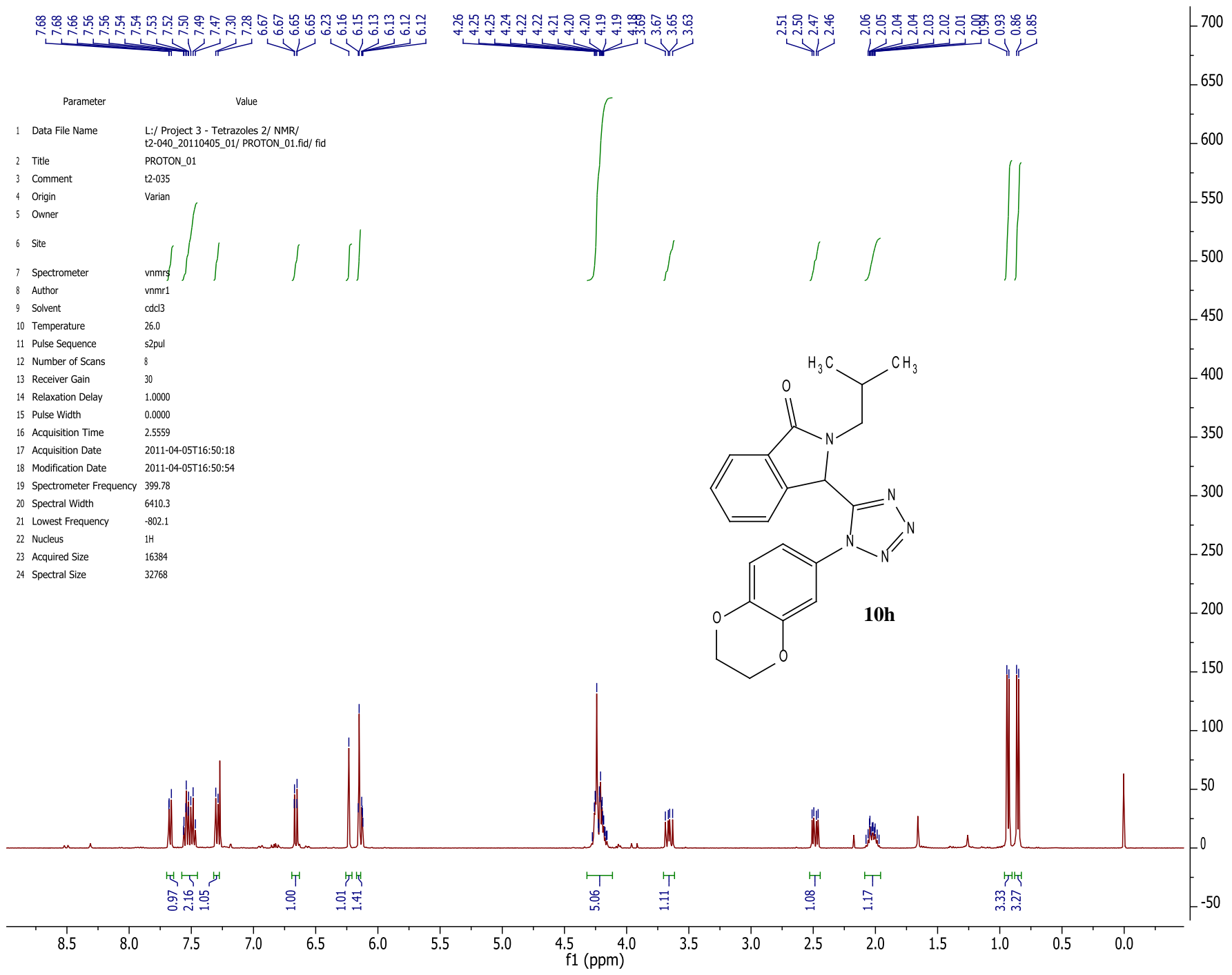






Parameter	Value
1 Data File Name	L:/ Project 3 - Tetrazoles 2/ NMR/ t2-039_20110405_01/ PROTON_01.fid/ fid
2 Title	PROTON_01
3 Comment	t2-035
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	vnmr1
9 Solvent	cdcl3
10 Temperature	26.0
11 Pulse Sequence	s2pul
12 Number of Scans	8
13 Receiver Gain	30
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	2.5559
17 Acquisition Date	2011-04-05T16:37:27
18 Modification Date	2011-04-05T16:38:02
19 Spectrometer Frequency	399.78
20 Spectral Width	6410.3
21 Lowest Frequency	-803.6
22 Nucleus	1H
23 Acquired Size	16384
24 Spectral Size	32768





Parameter Value

1 Data File Name L:/ Project 3 - Tetrazoles 2/ NMR/ t2-040_20110405_01/ PROTON_01.fid/ fid

2 Title PROTON_01

3 Comment t2-035

4 Origin Varian

5 Owner

6 Site

7 Spectrometer vnmr5

8 Author vnmr1

9 Solvent cdcl3

10 Temperature 26.0

11 Pulse Sequence s2pul

12 Number of Scans 8

13 Receiver Gain 30

14 Relaxation Delay 1.0000

15 Pulse Width 0.0000

16 Acquisition Time 2.5559

17 Acquisition Date 2011-04-05T16:50:18

18 Modification Date 2011-04-05T16:50:54

19 Spectrometer Frequency 399.78

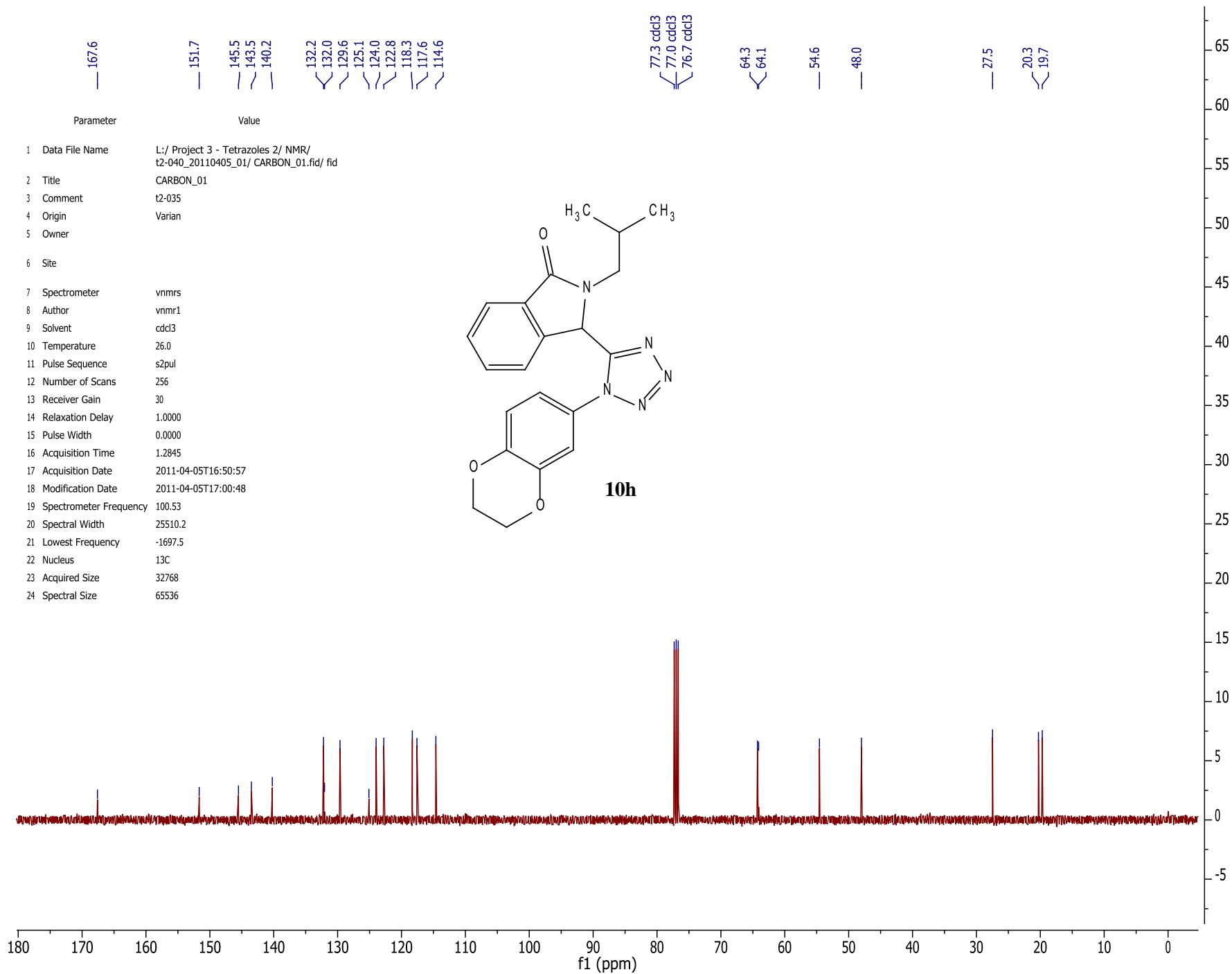
20 Spectral Width 6410.3

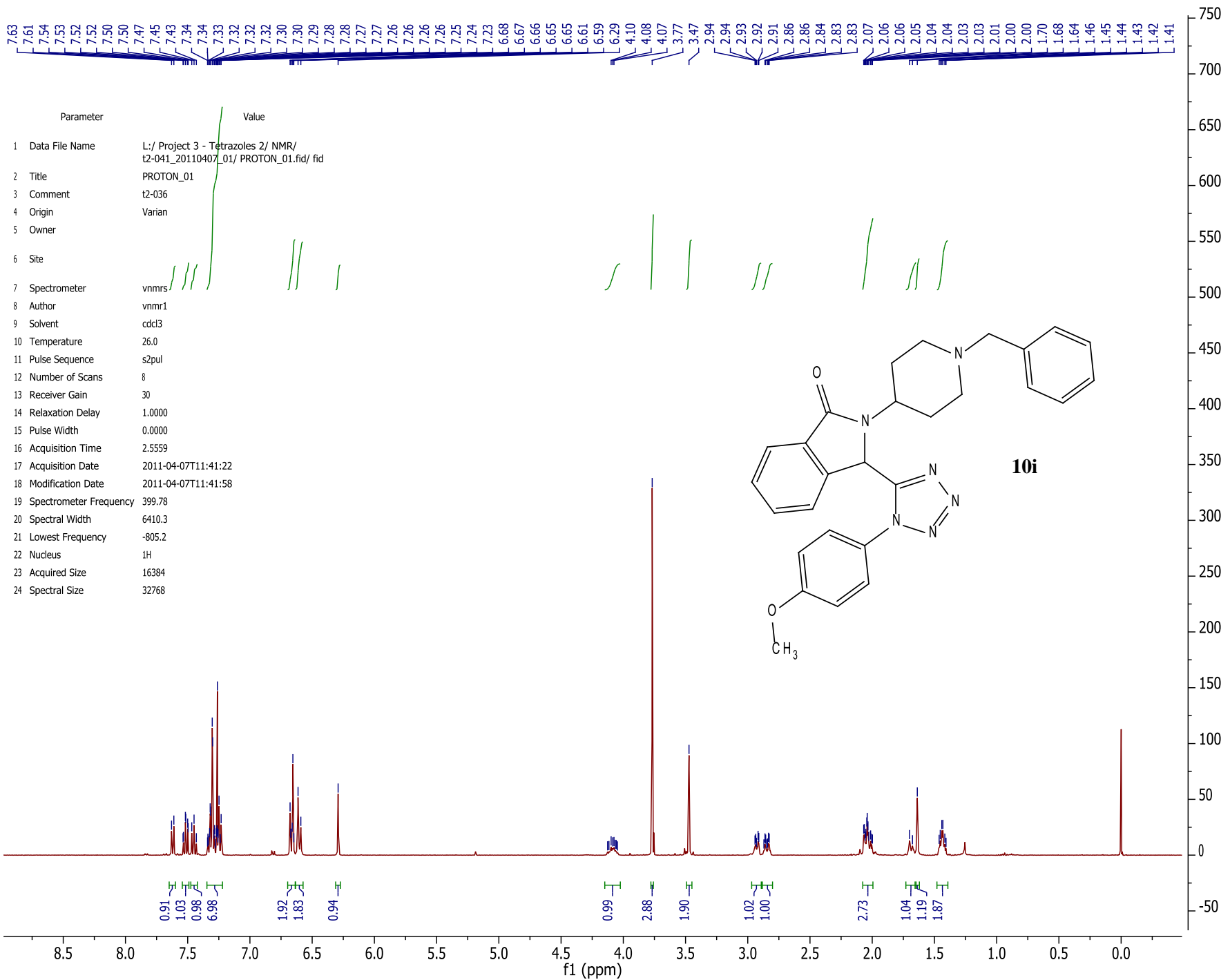
21 Lowest Frequency -802.1

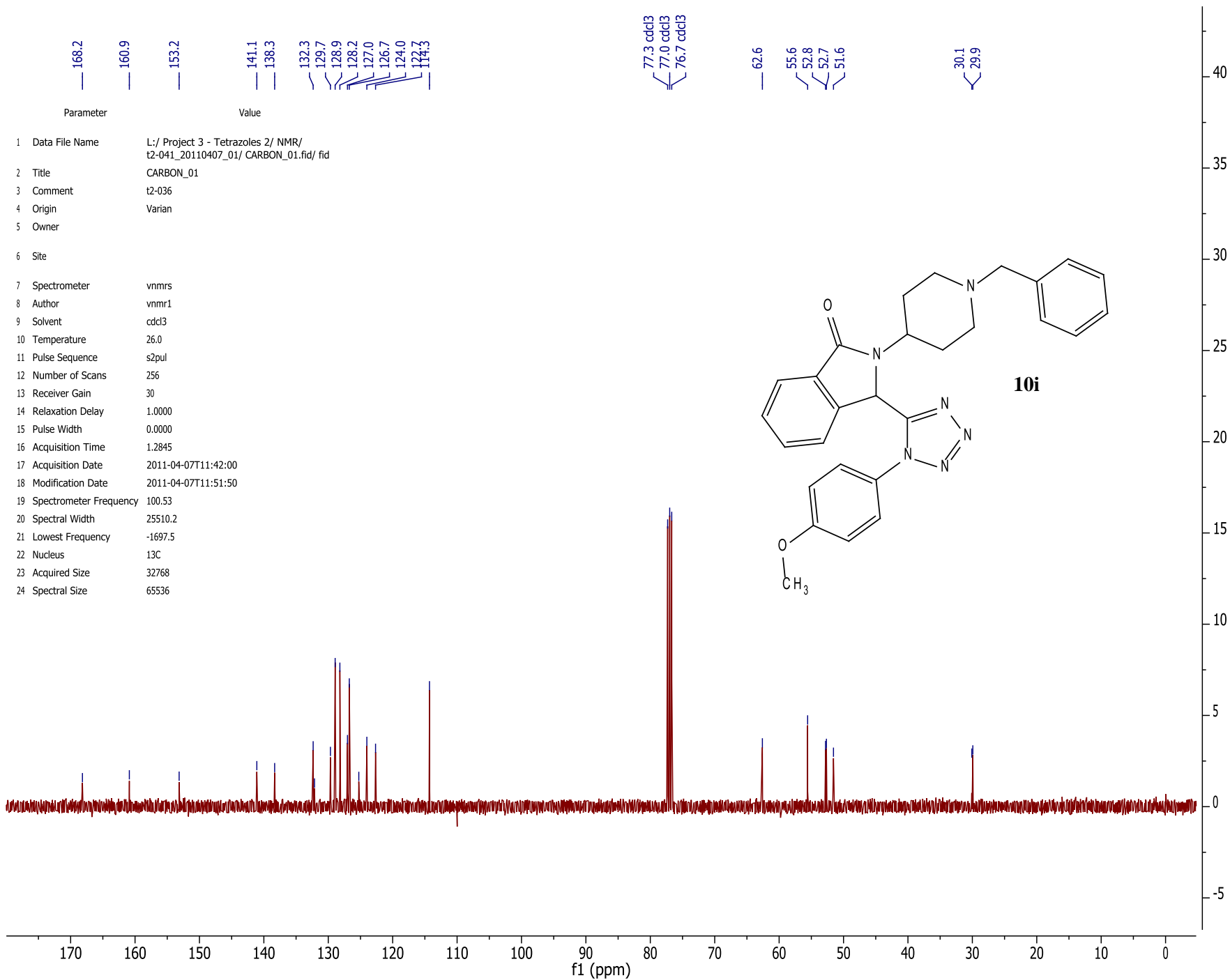
22 Nucleus 1H

23 Acquired Size 16384

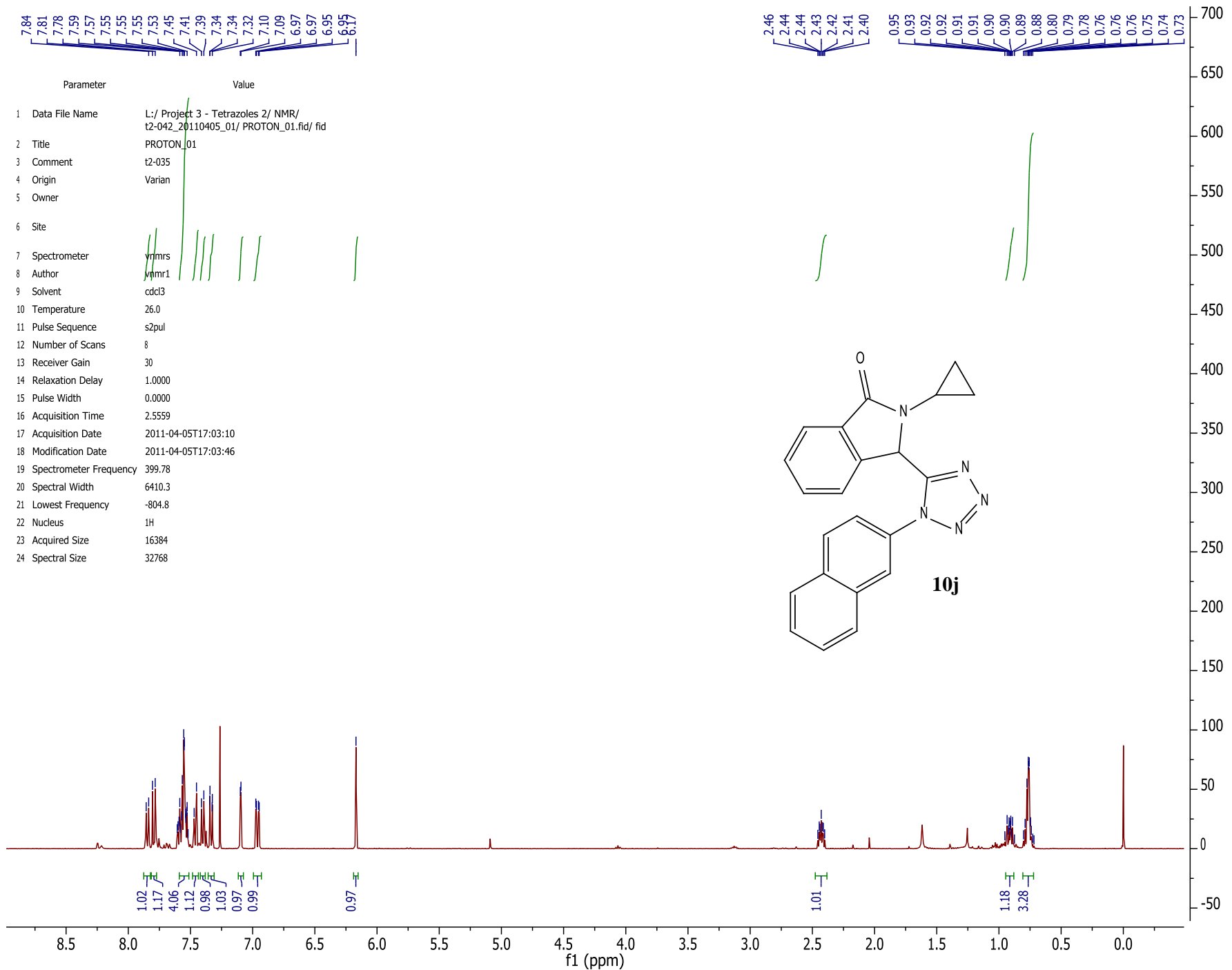
24 Spectral Size 32768



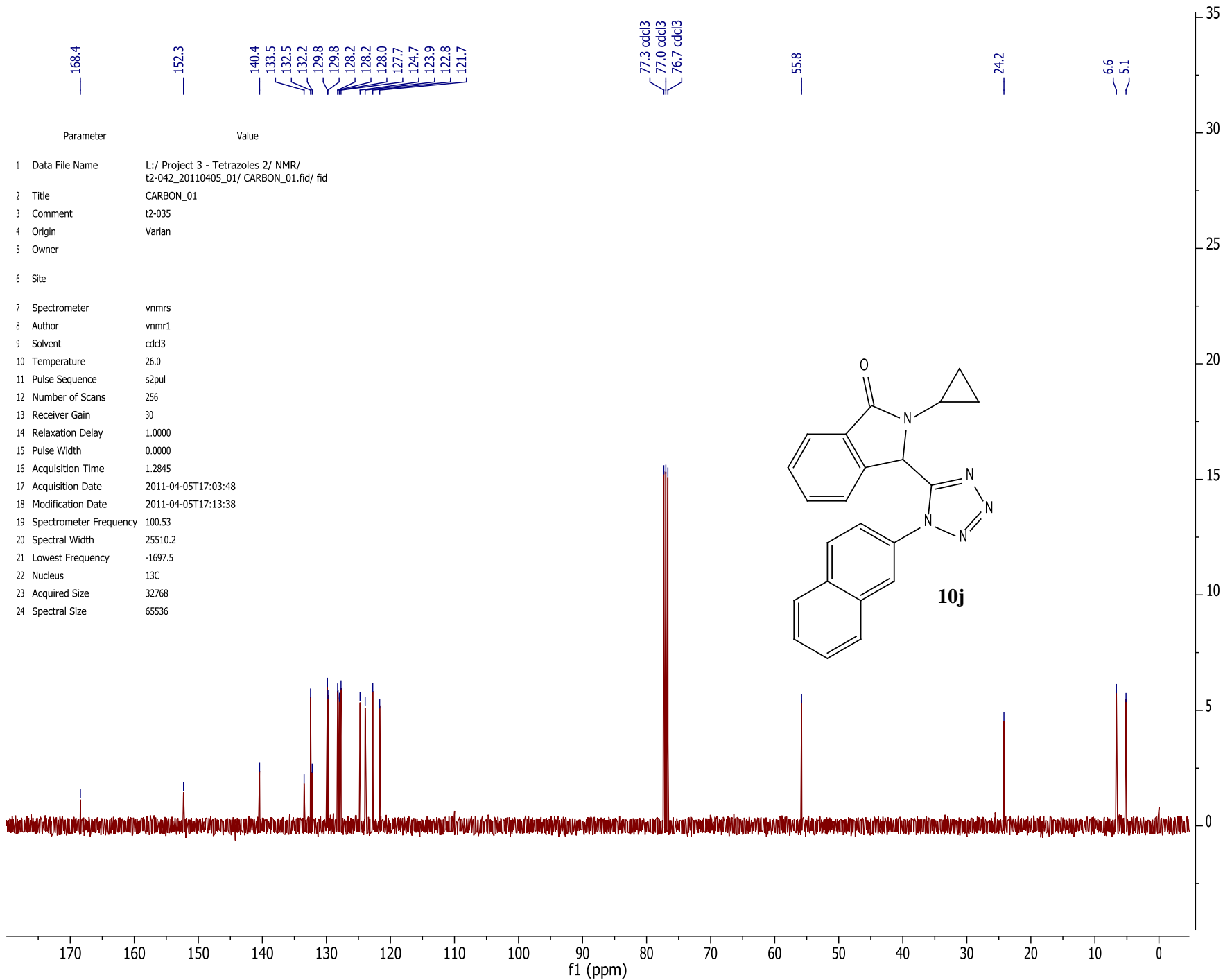




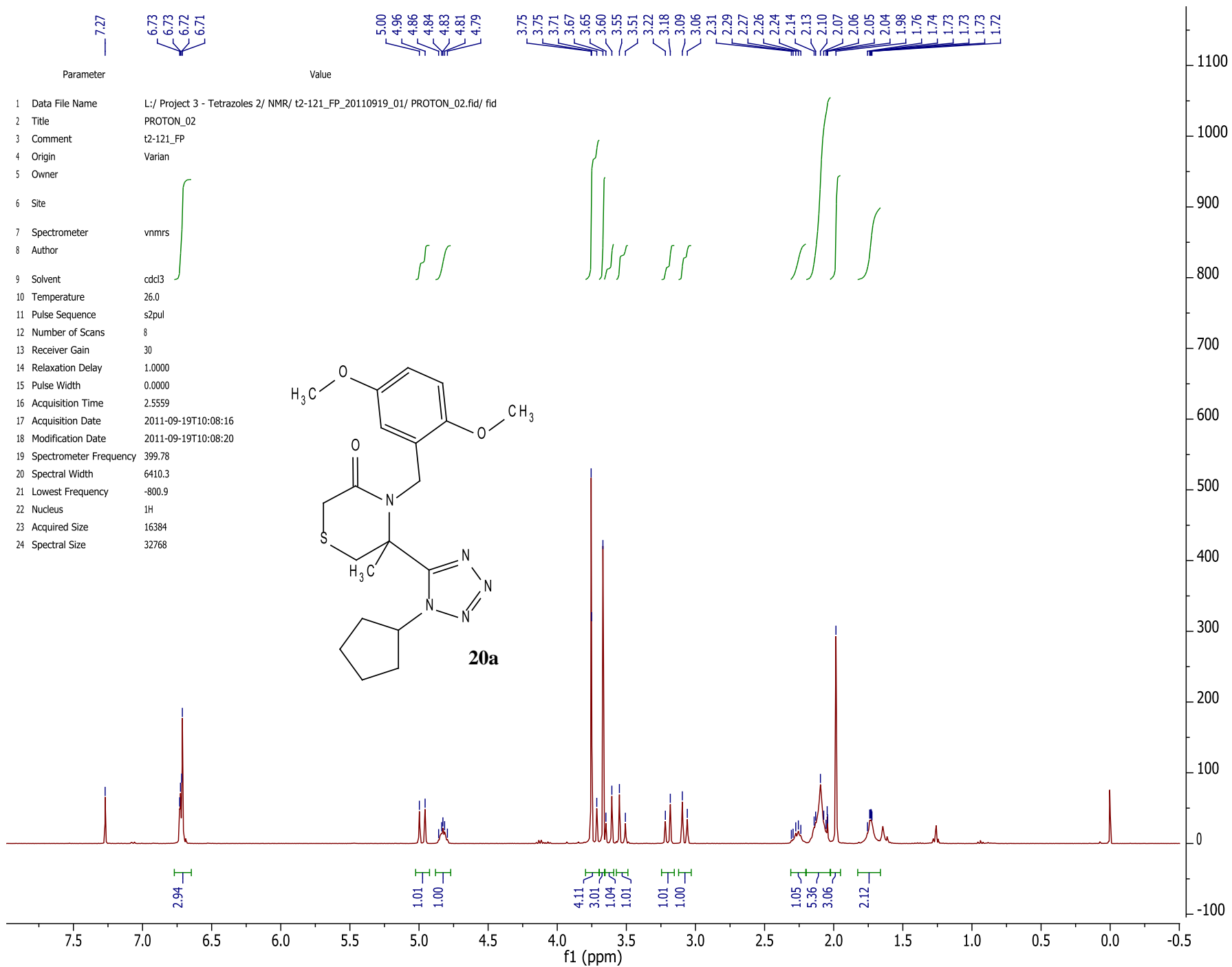
Parameter	Value
1 Data File Name	L:/ Project 3 - Tetrazoles 2/ NMR/ t2-041_20110407_01/ CARBON_01.fid/ fid
2 Title	CARBON_01
3 Comment	t2-036
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	vnmr1
9 Solvent	cdcl3
10 Temperature	26.0
11 Pulse Sequence	s2pul
12 Number of Scans	256
13 Receiver Gain	30
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.2845
17 Acquisition Date	2011-04-07T11:42:00
18 Modification Date	2011-04-07T11:51:50
19 Spectrometer Frequency	100.53
20 Spectral Width	25510.2
21 Lowest Frequency	-1697.5
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

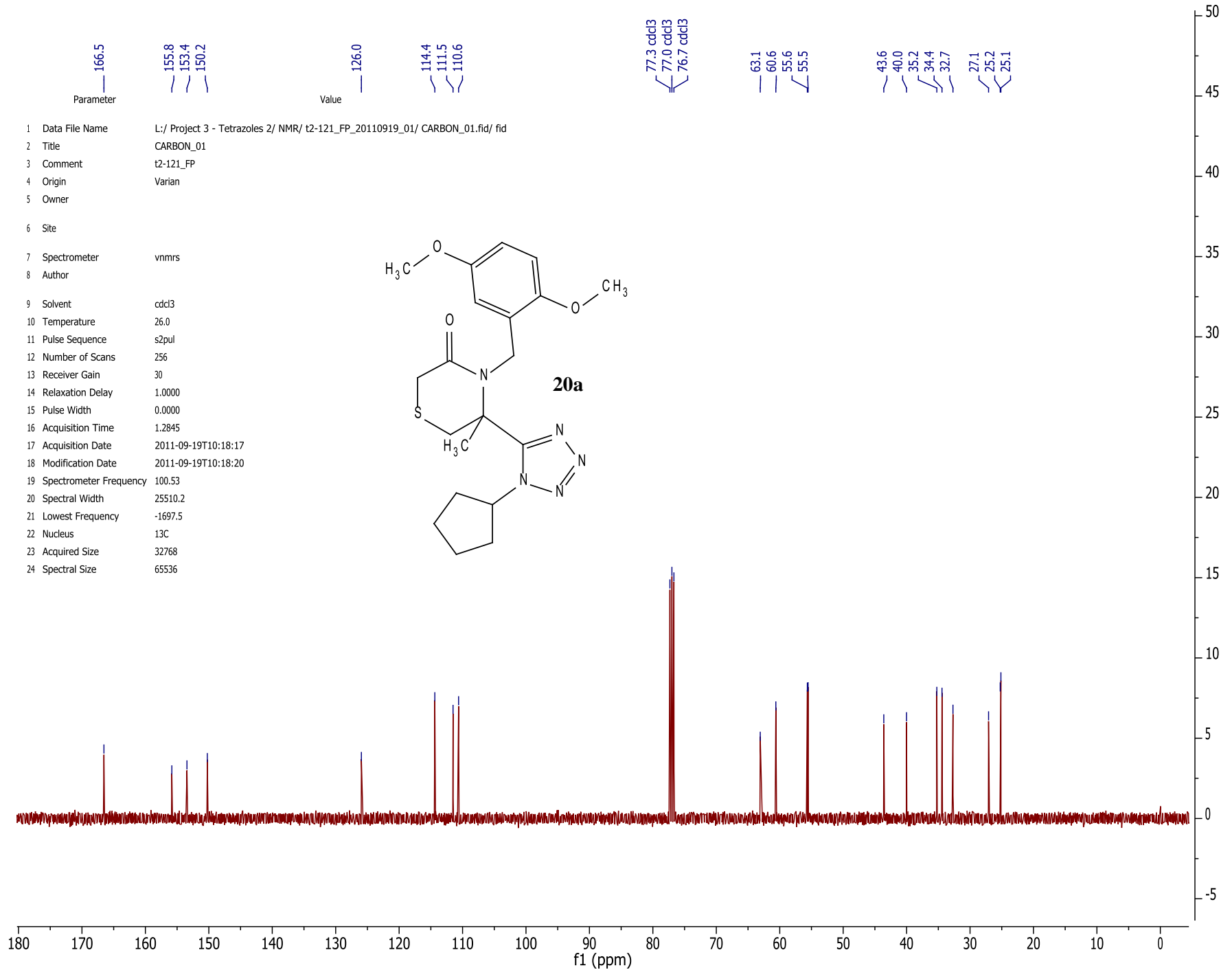


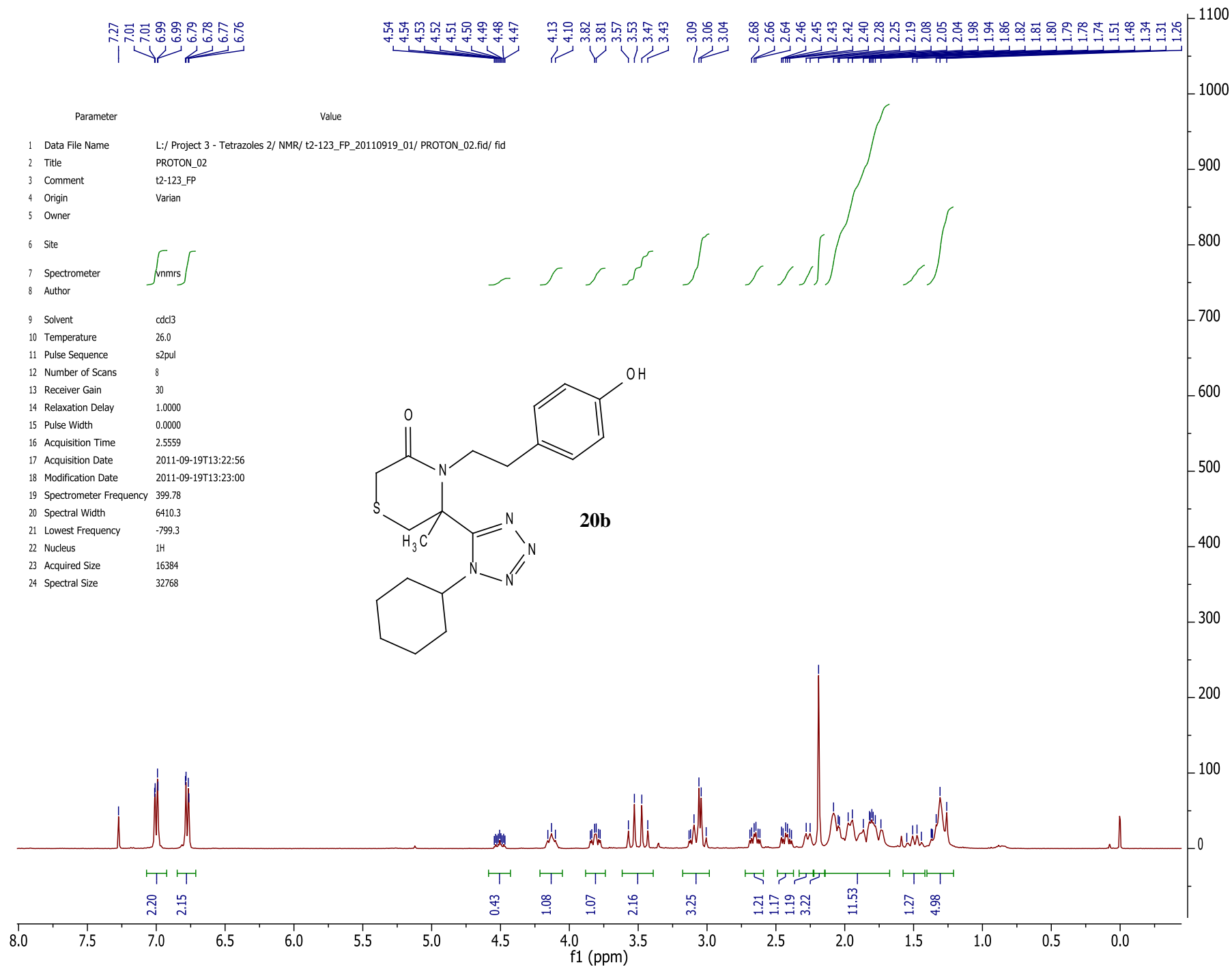
Parameter	Value
1 Data File Name	L:/ Project 3 - Tetrazoles 2/ NMR/ t2-042_20110405_01/ PROTON_01.fid/ fid
2 Title	PROTON_01
3 Comment	t2-035
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	ymrms
8 Author	ymr1
9 Solvent	cdcl3
10 Temperature	26.0
11 Pulse Sequence	s2pul
12 Number of Scans	8
13 Receiver Gain	30
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	2.5559
17 Acquisition Date	2011-04-05T17:03:10
18 Modification Date	2011-04-05T17:03:46
19 Spectrometer Frequency	399.78
20 Spectral Width	6410.3
21 Lowest Frequency	-804.8
22 Nucleus	1H
23 Acquired Size	16384
24 Spectral Size	32768

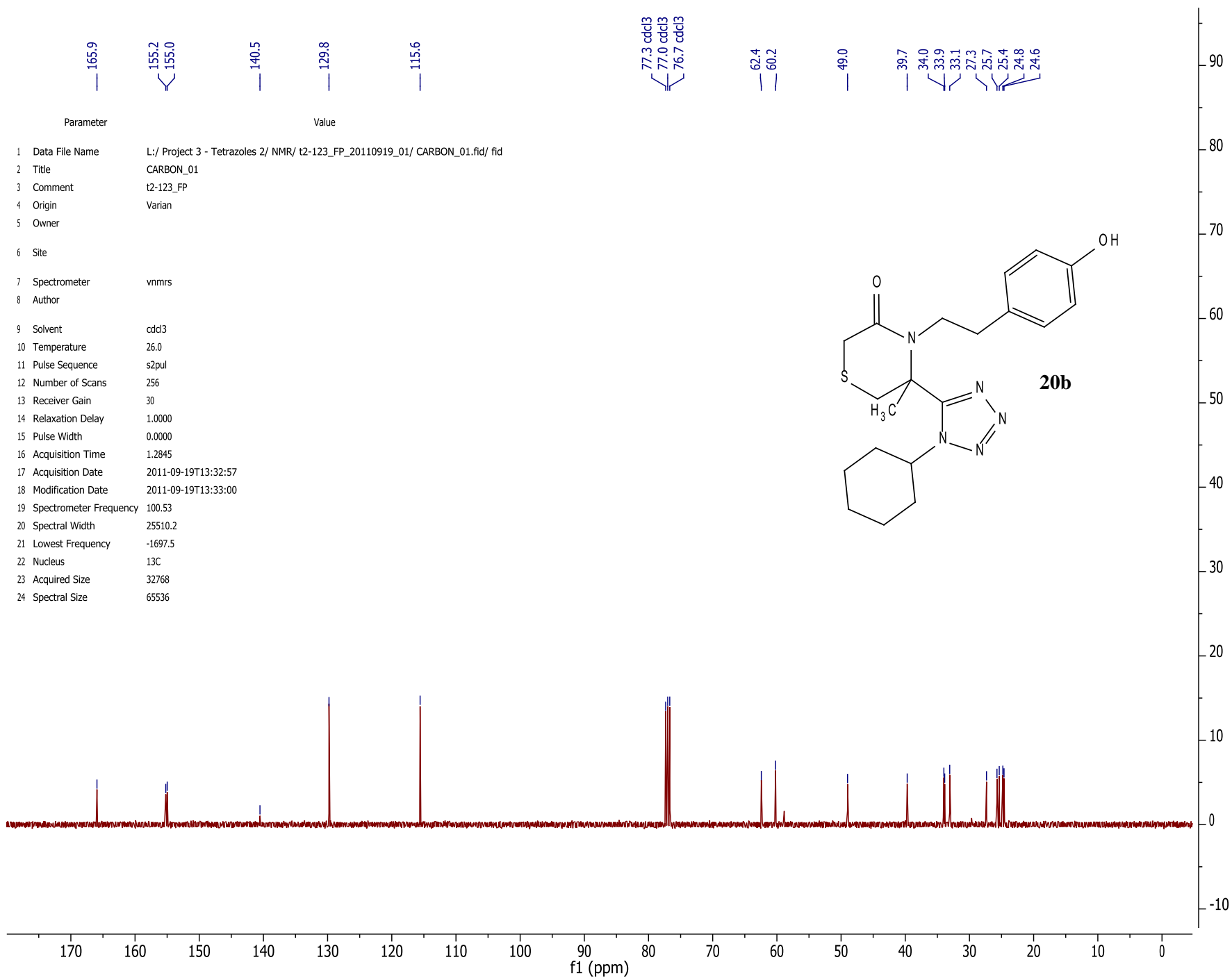


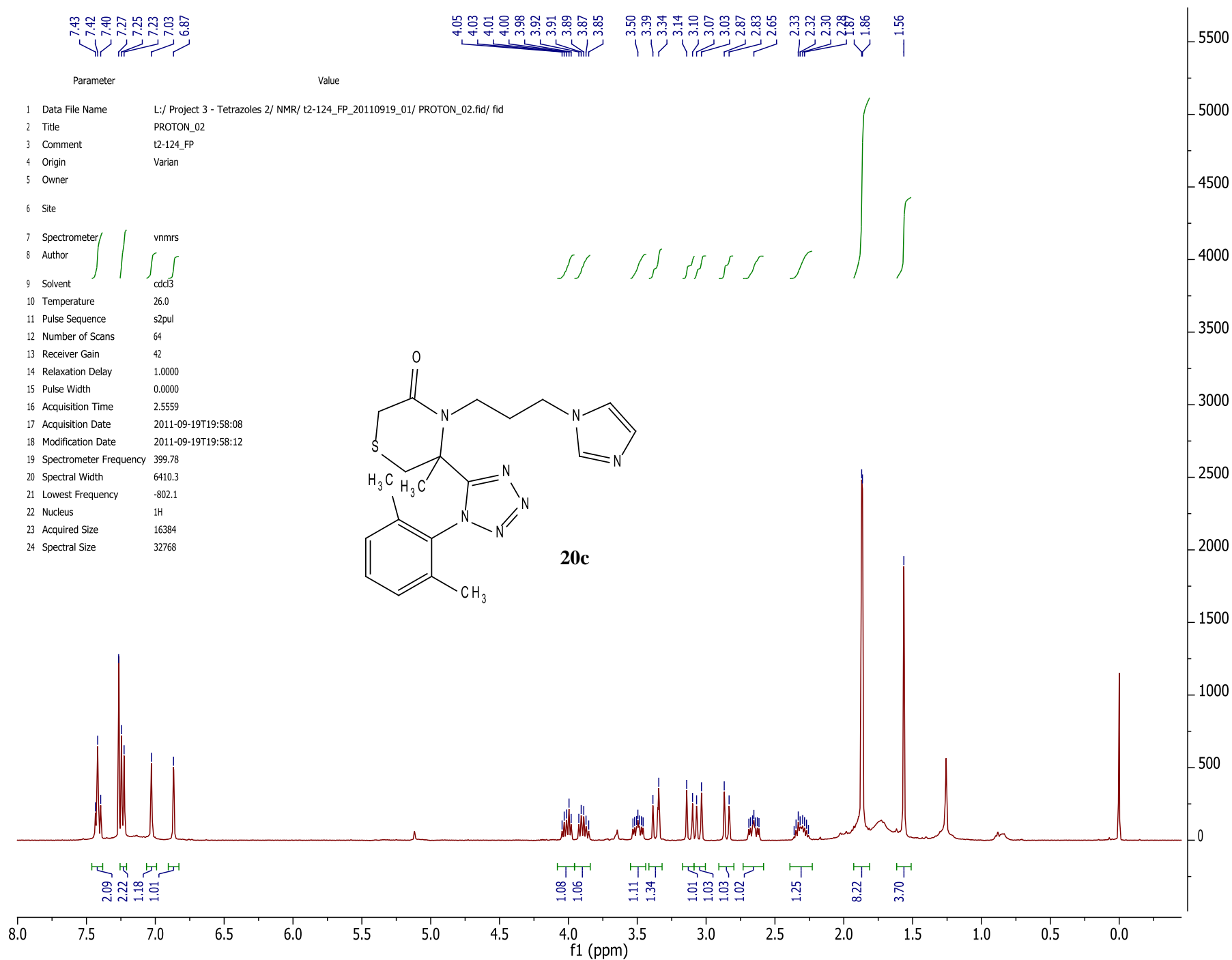
Parameter	Value
1 Data File Name	L:/ Project 3 - Tetrazoles 2/ NMR/ t2-042_20110405_01/ CARBON_01.fid/ fid
2 Title	CARBON_01
3 Comment	t2-035
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	vnmr1
9 Solvent	cdcl3
10 Temperature	26.0
11 Pulse Sequence	s2pul
12 Number of Scans	256
13 Receiver Gain	30
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.2845
17 Acquisition Date	2011-04-05T17:03:48
18 Modification Date	2011-04-05T17:13:38
19 Spectrometer Frequency	100.53
20 Spectral Width	25510.2
21 Lowest Frequency	-1697.5
22 Nucleus	¹³ C
23 Acquired Size	32768
24 Spectral Size	65536

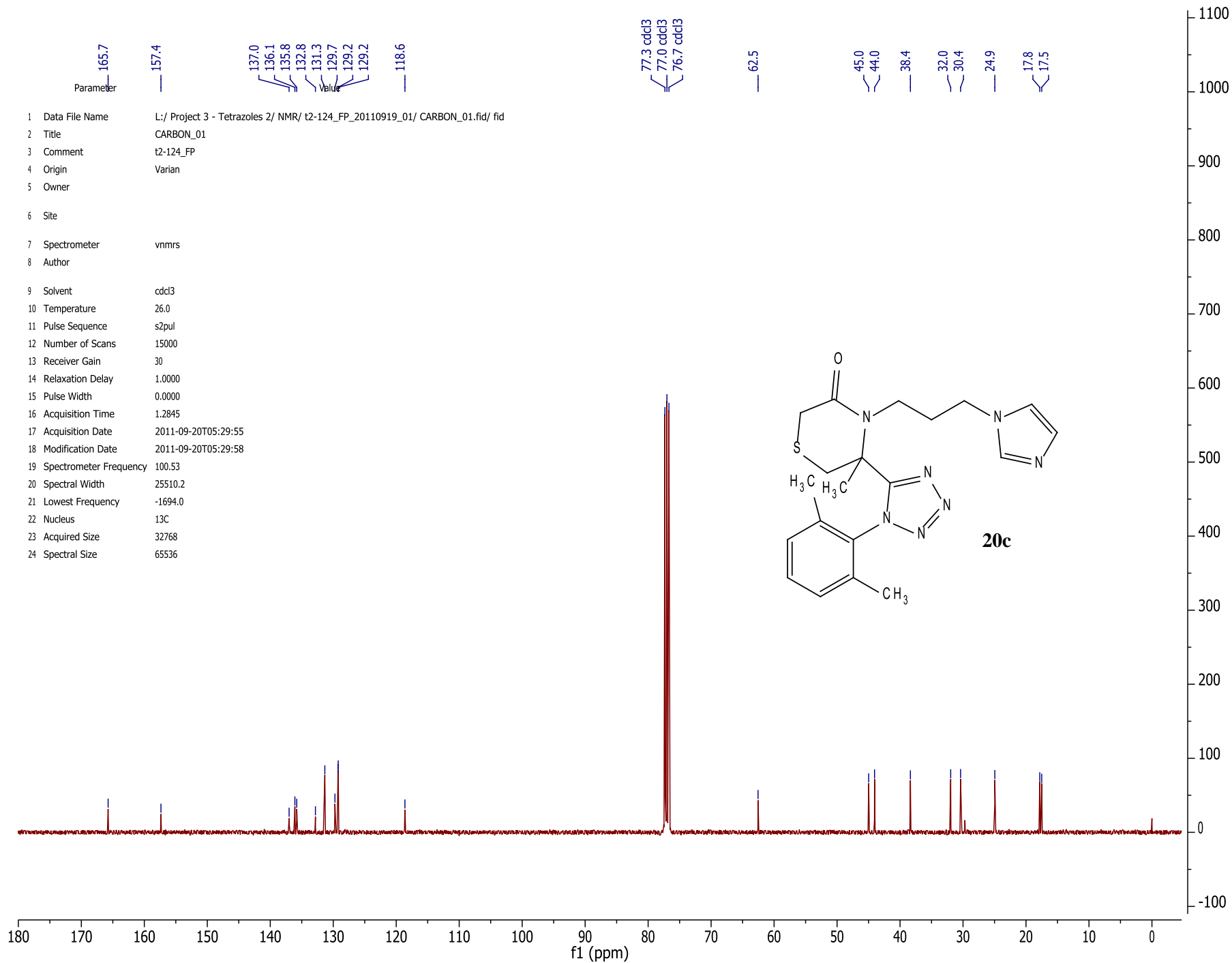


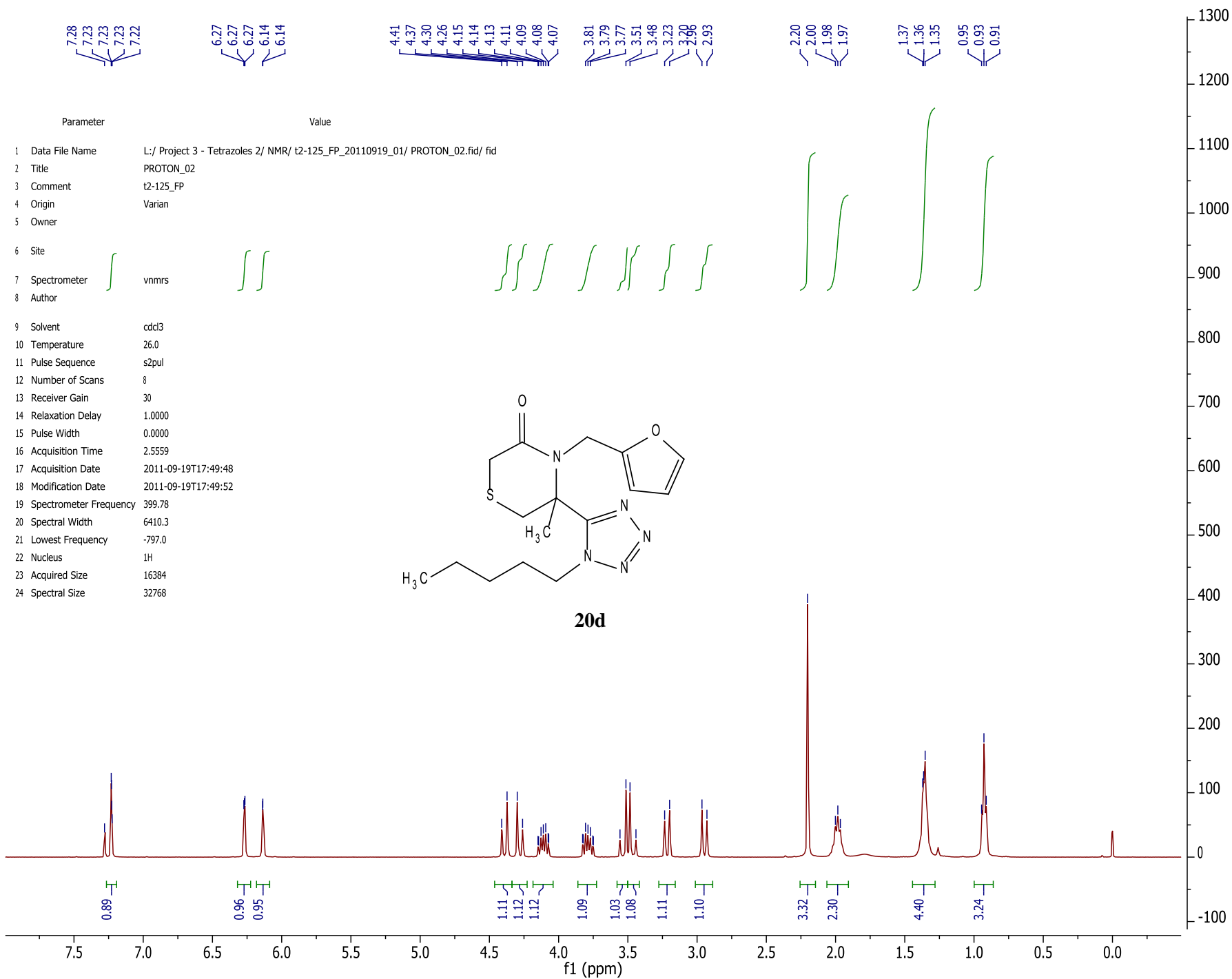


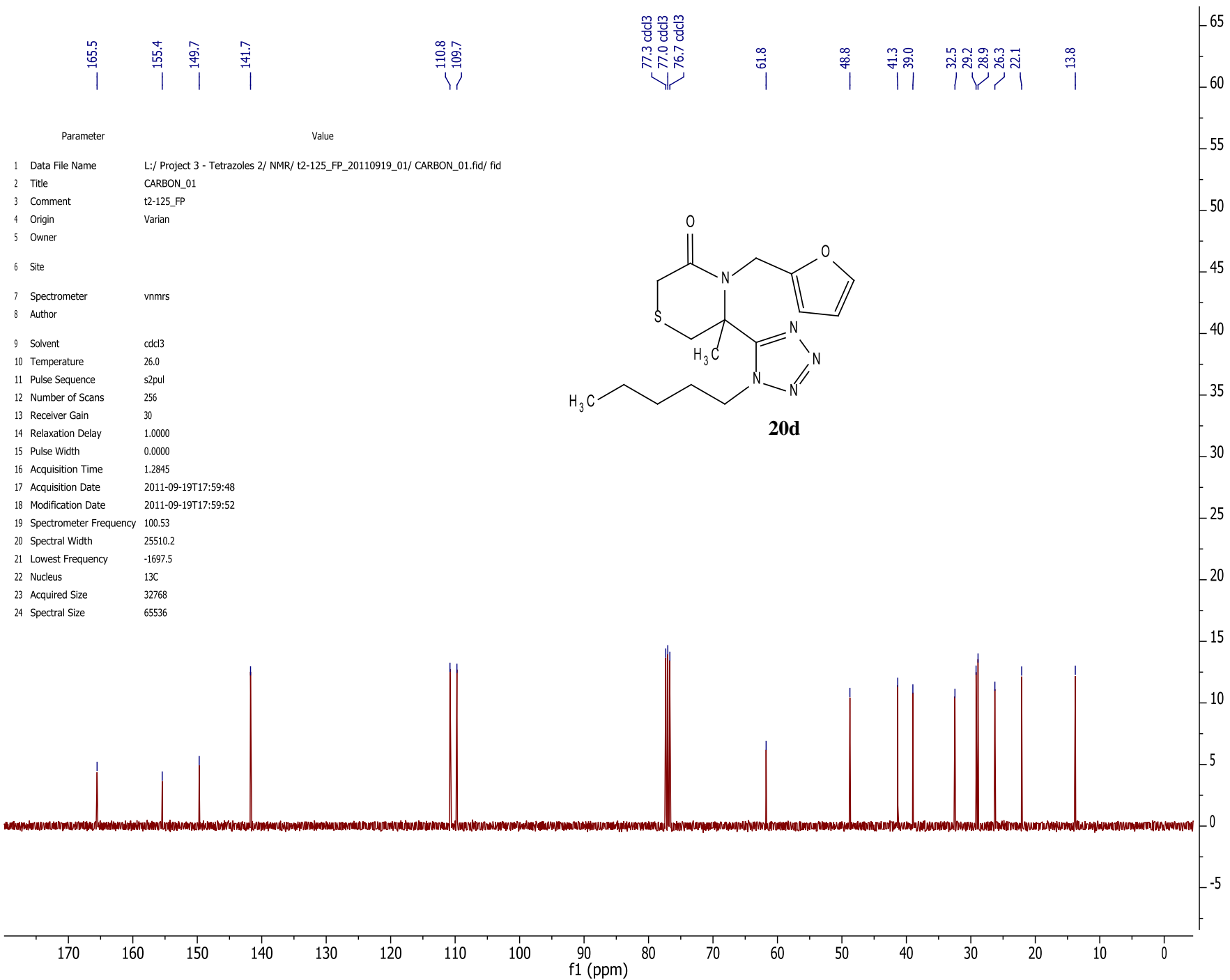


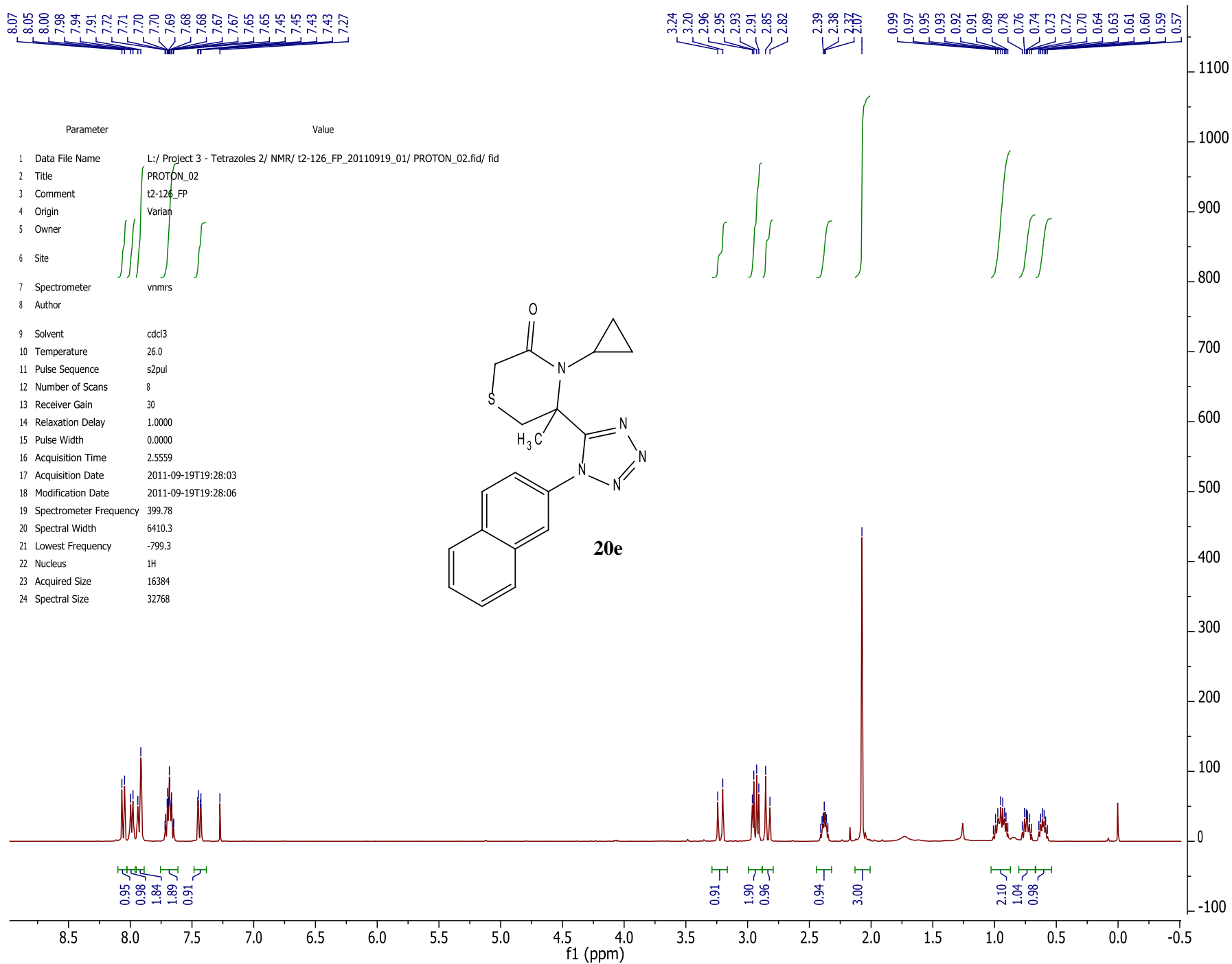




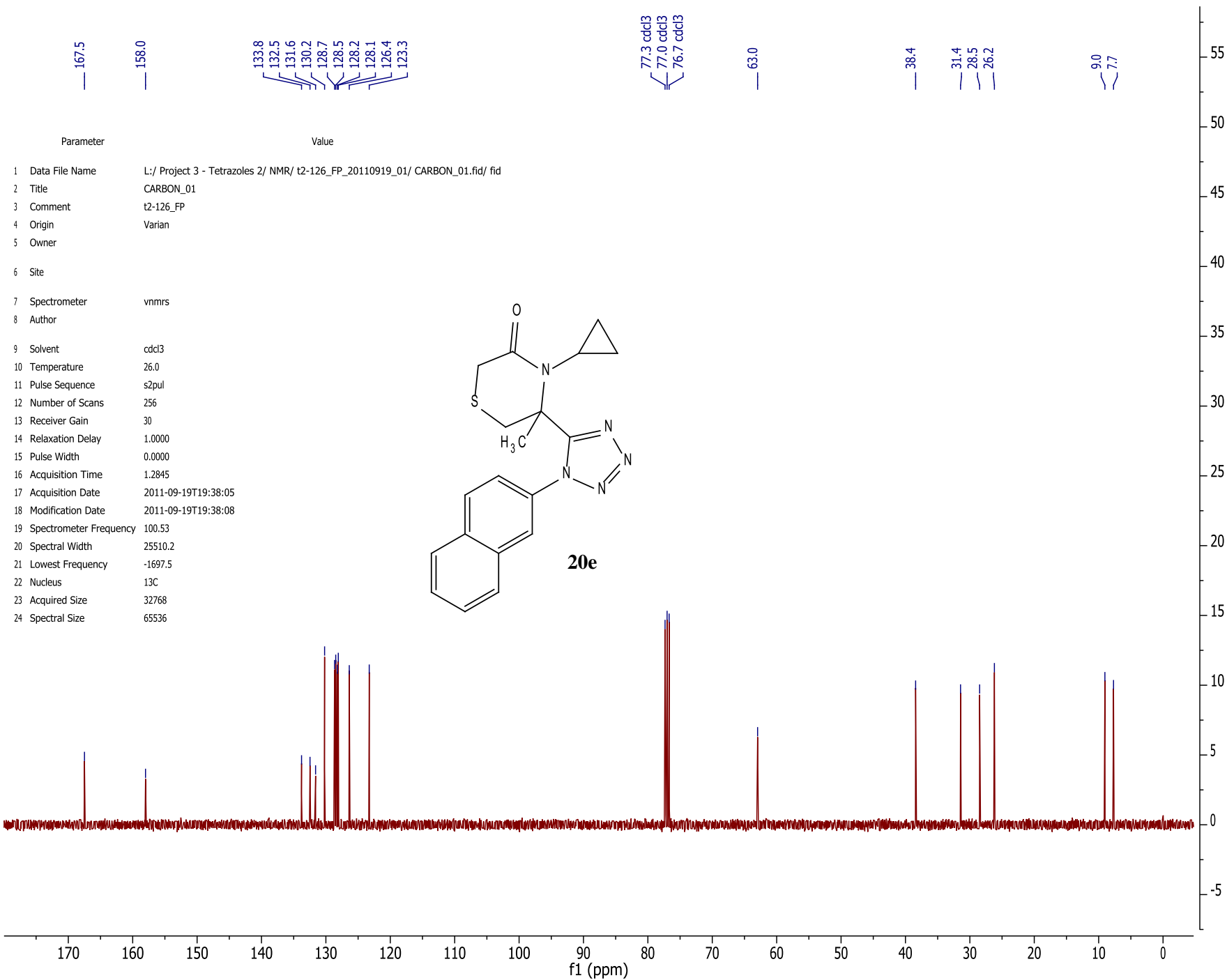




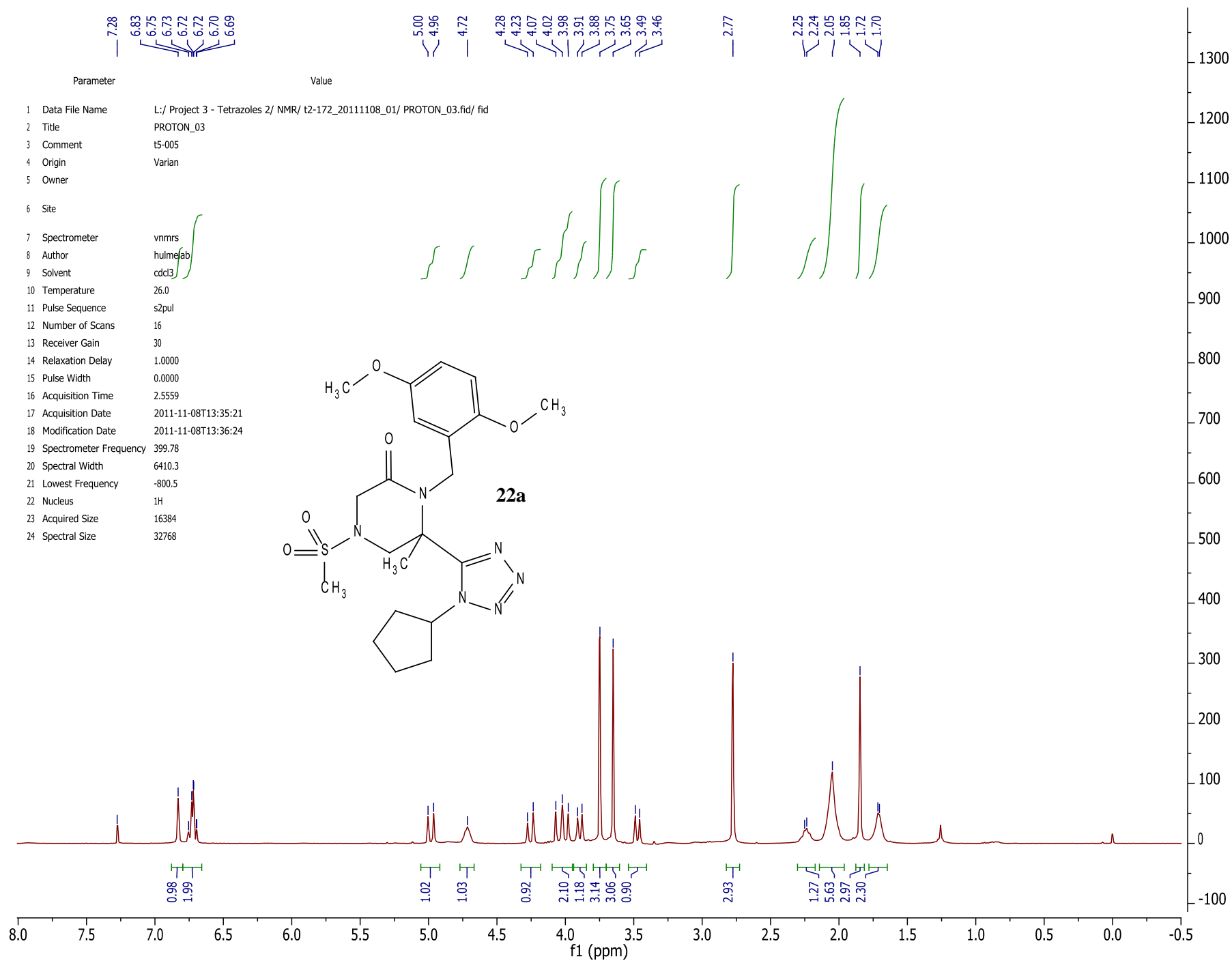


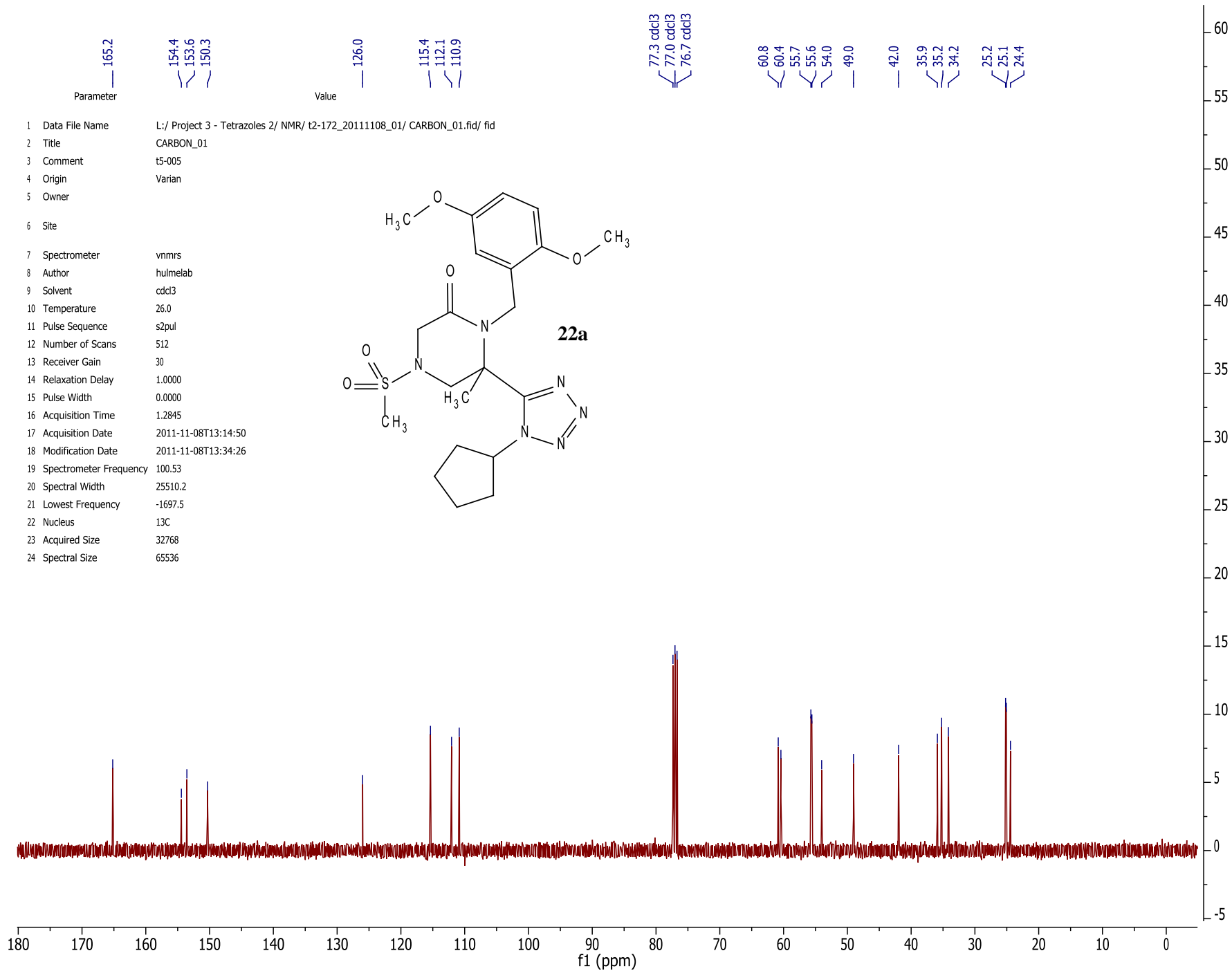


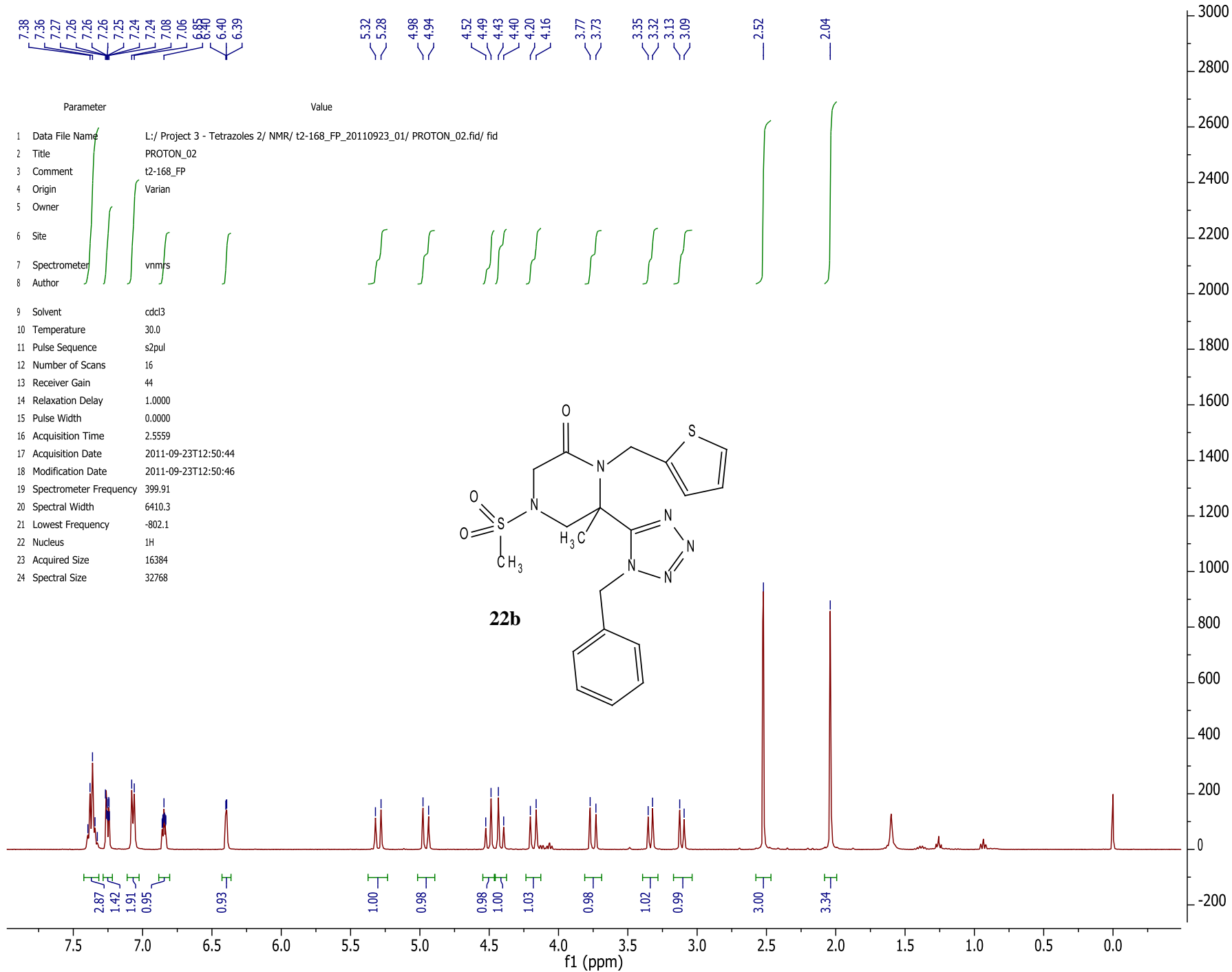
Parameter	Value
1 Data File Name	L:/ Project 3 - Tetrazoles 2/ NMR/ t2-126_FP_20110919_01/ PROTON_02.fid/ fid
2 Title	PROTON_02
3 Comment	t2-126_FP
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnms
8 Author	
9 Solvent	cdcl3
10 Temperature	26.0
11 Pulse Sequence	s2pul
12 Number of Scans	8
13 Receiver Gain	30
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	2.5559
17 Acquisition Date	2011-09-19T19:28:03
18 Modification Date	2011-09-19T19:28:06
19 Spectrometer Frequency	399.78
20 Spectral Width	6410.3
21 Lowest Frequency	-799.3
22 Nucleus	1H
23 Acquired Size	16384
24 Spectral Size	32768

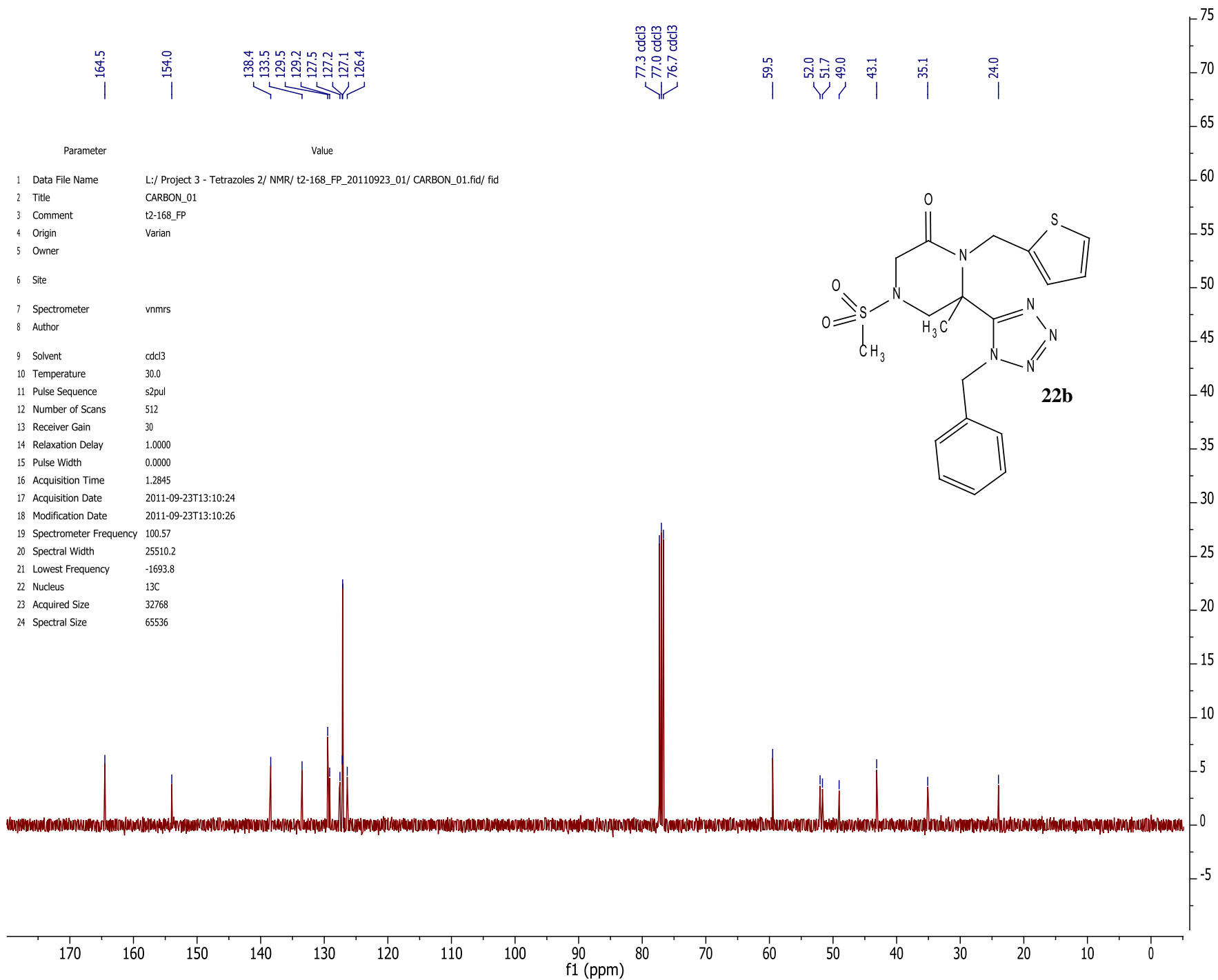


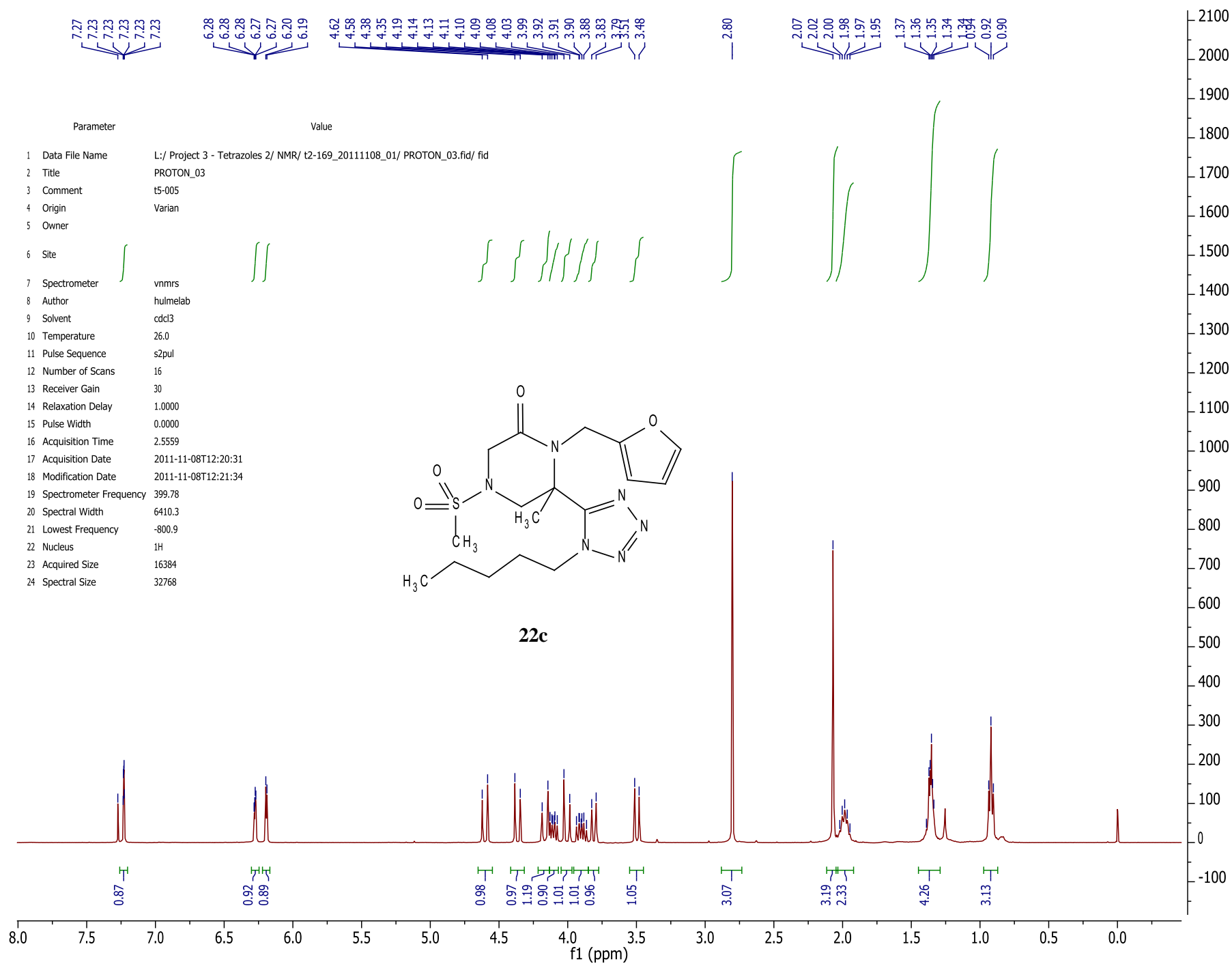
Parameter	Value
1 Data File Name	L:/ Project 3 - Tetrazoles 2/ NMR/ t2-126_FP_20110919_01/ CARBON_01.fid/ fid
2 Title	CARBON_01
3 Comment	t2-126_FP
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	nmrs
8 Author	
9 Solvent	cdcl3
10 Temperature	26.0
11 Pulse Sequence	s2pul
12 Number of Scans	256
13 Receiver Gain	30
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.2845
17 Acquisition Date	2011-09-19T19:38:05
18 Modification Date	2011-09-19T19:38:08
19 Spectrometer Frequency	100.53
20 Spectral Width	25510.2
21 Lowest Frequency	-1697.5
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

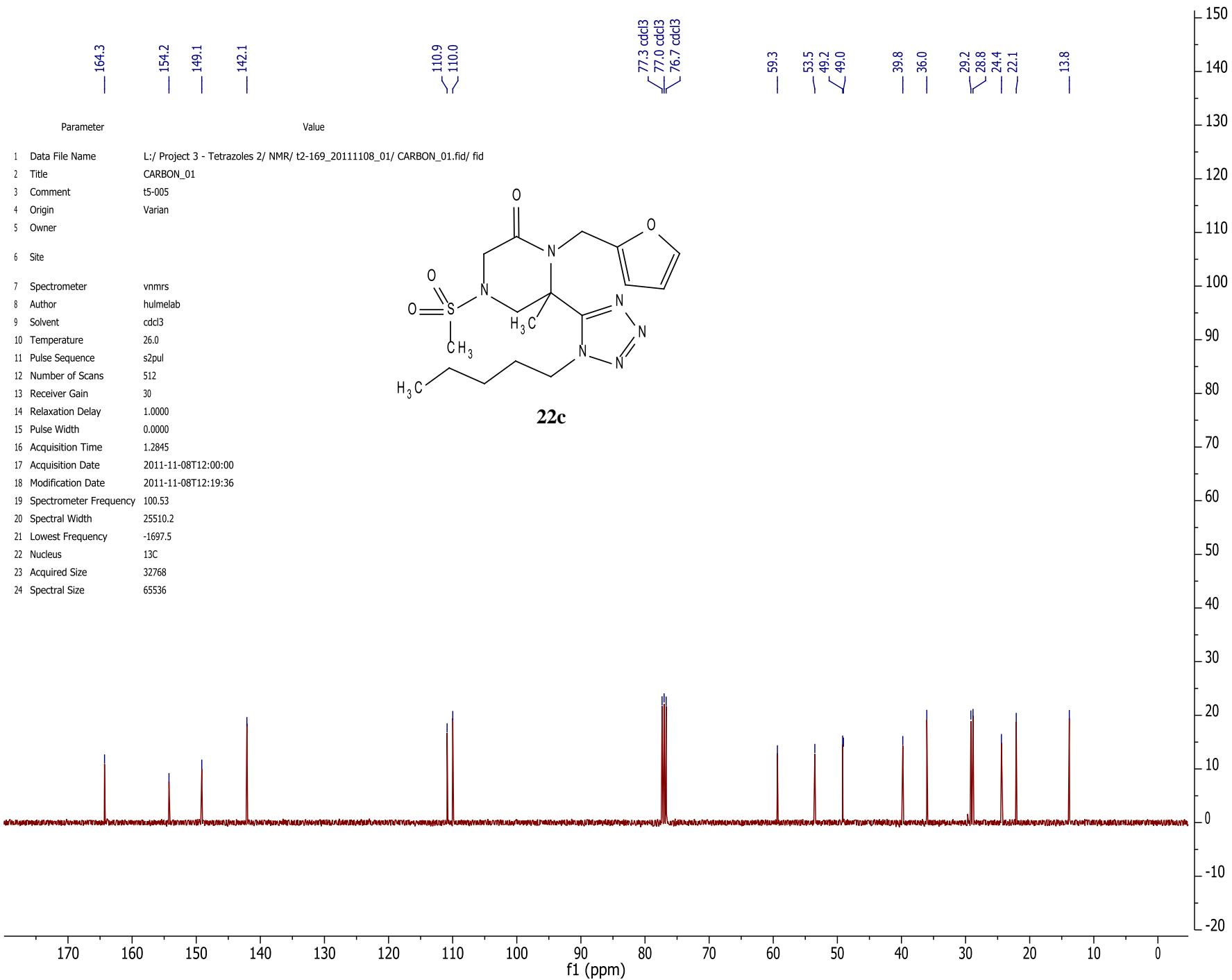


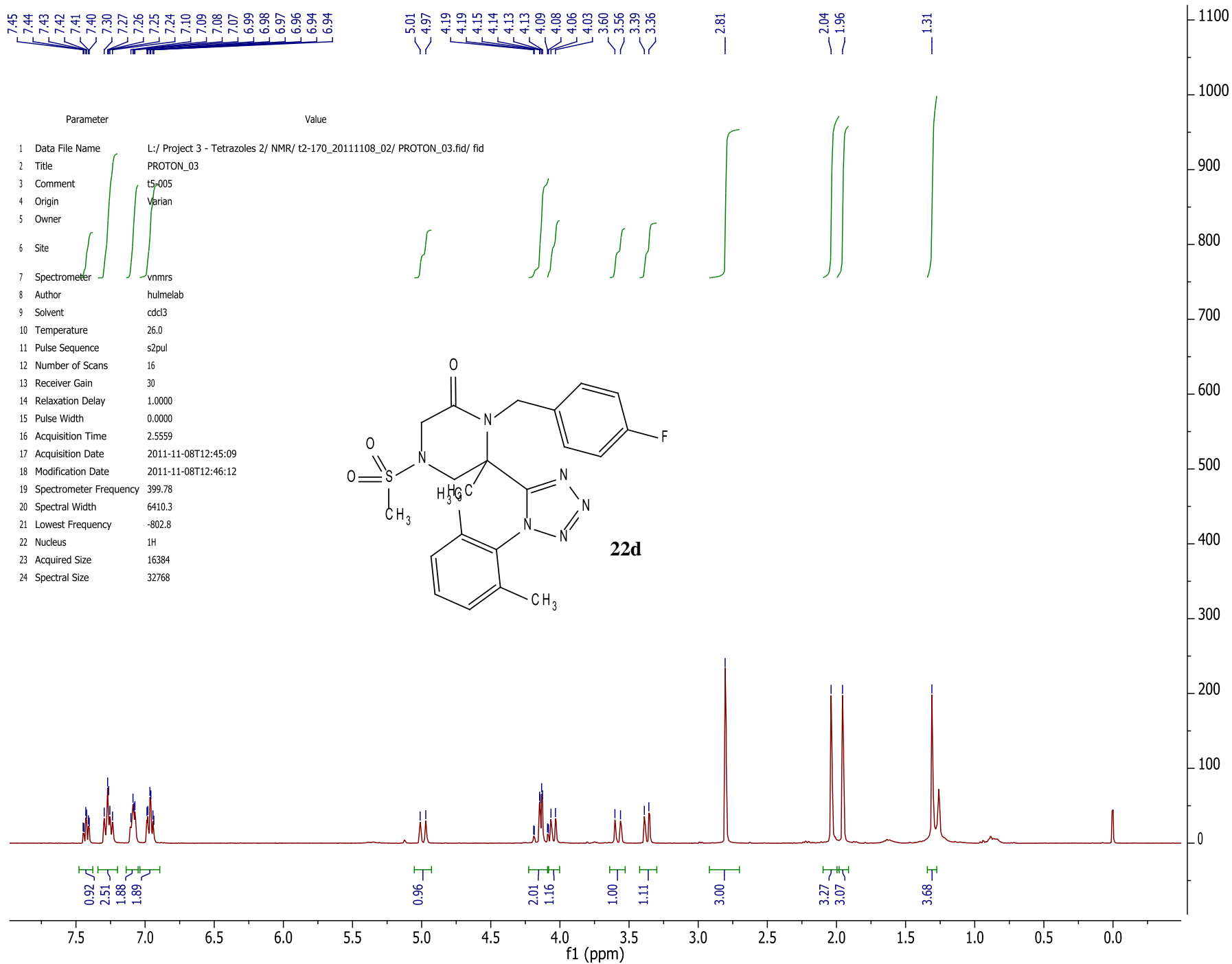


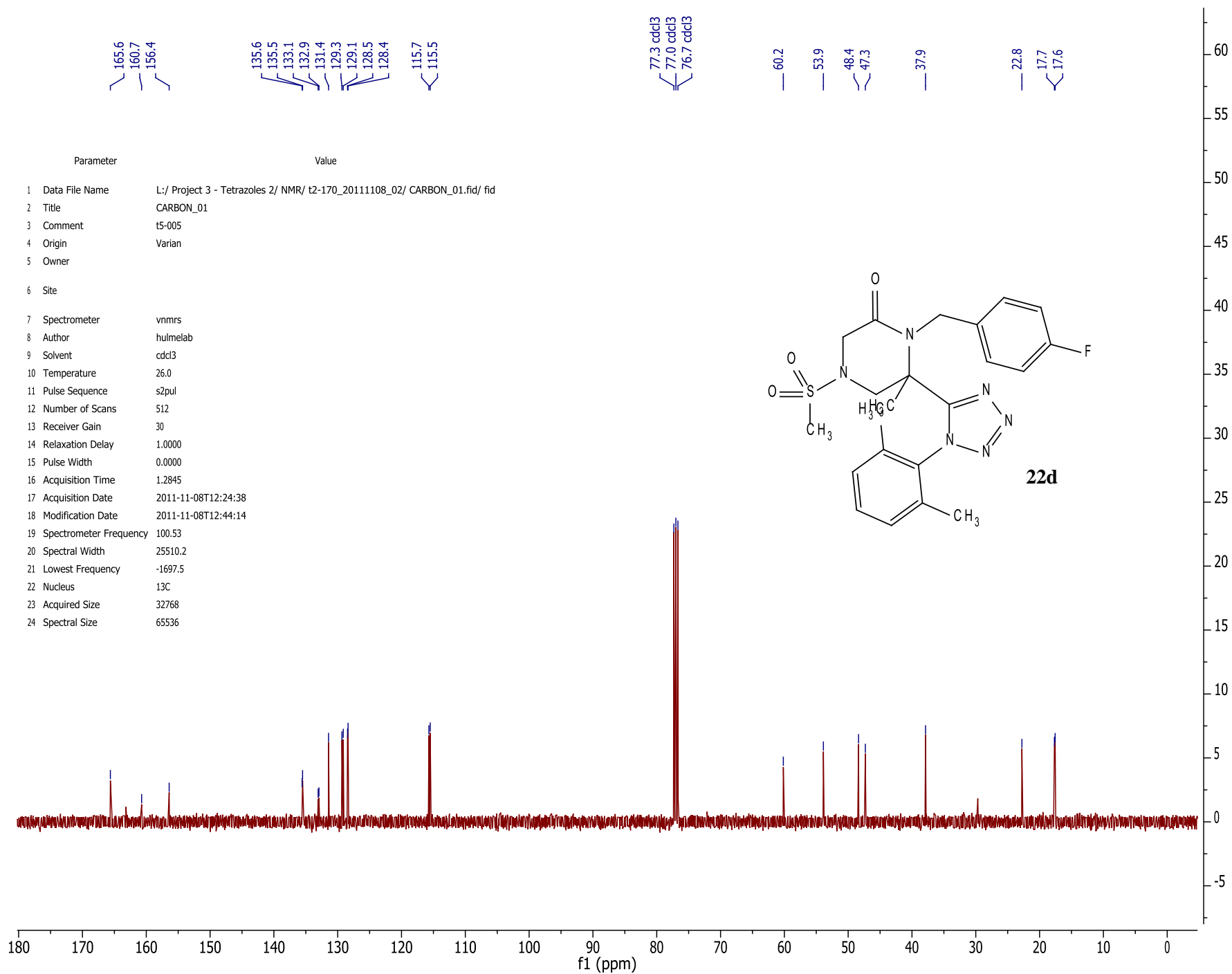


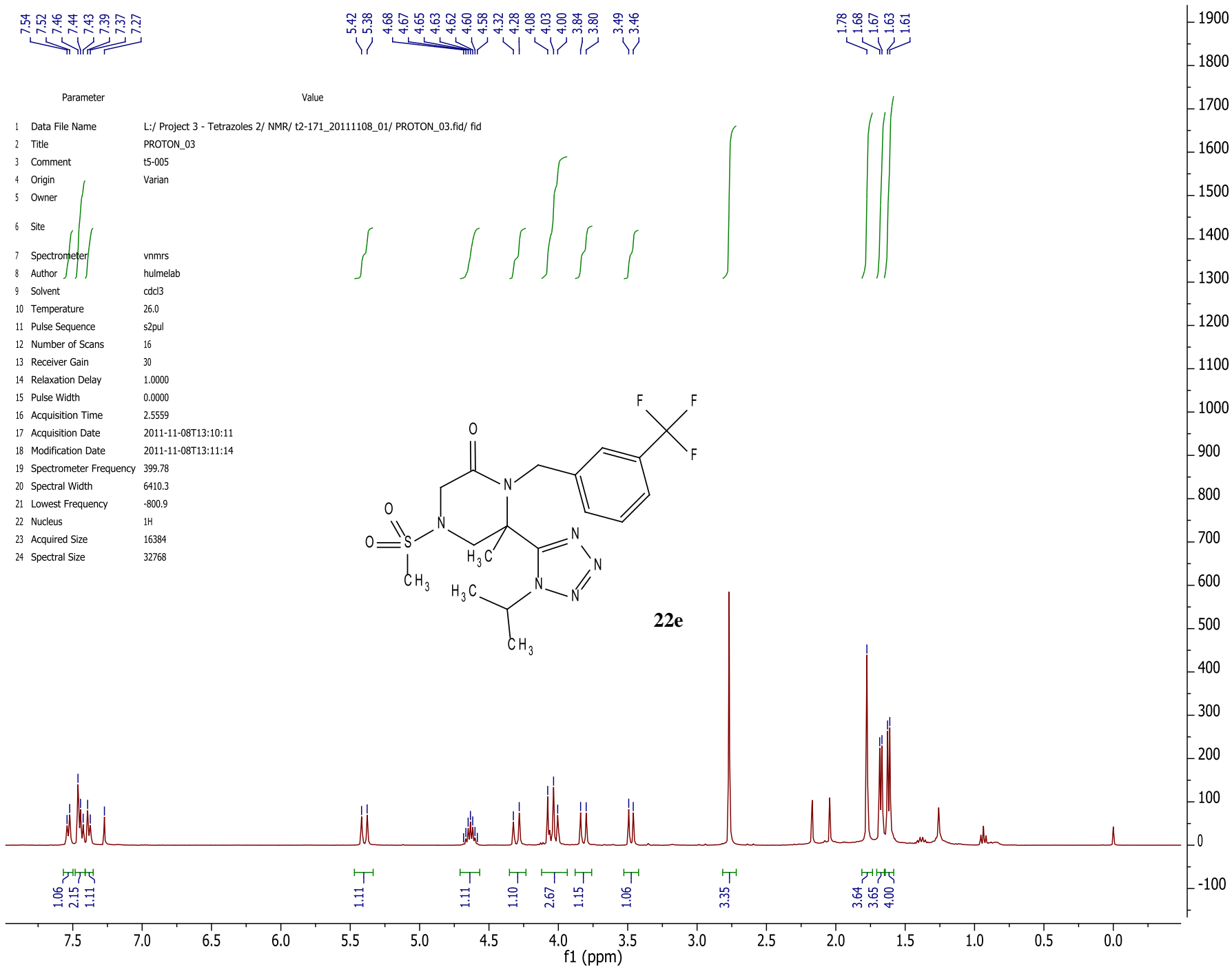


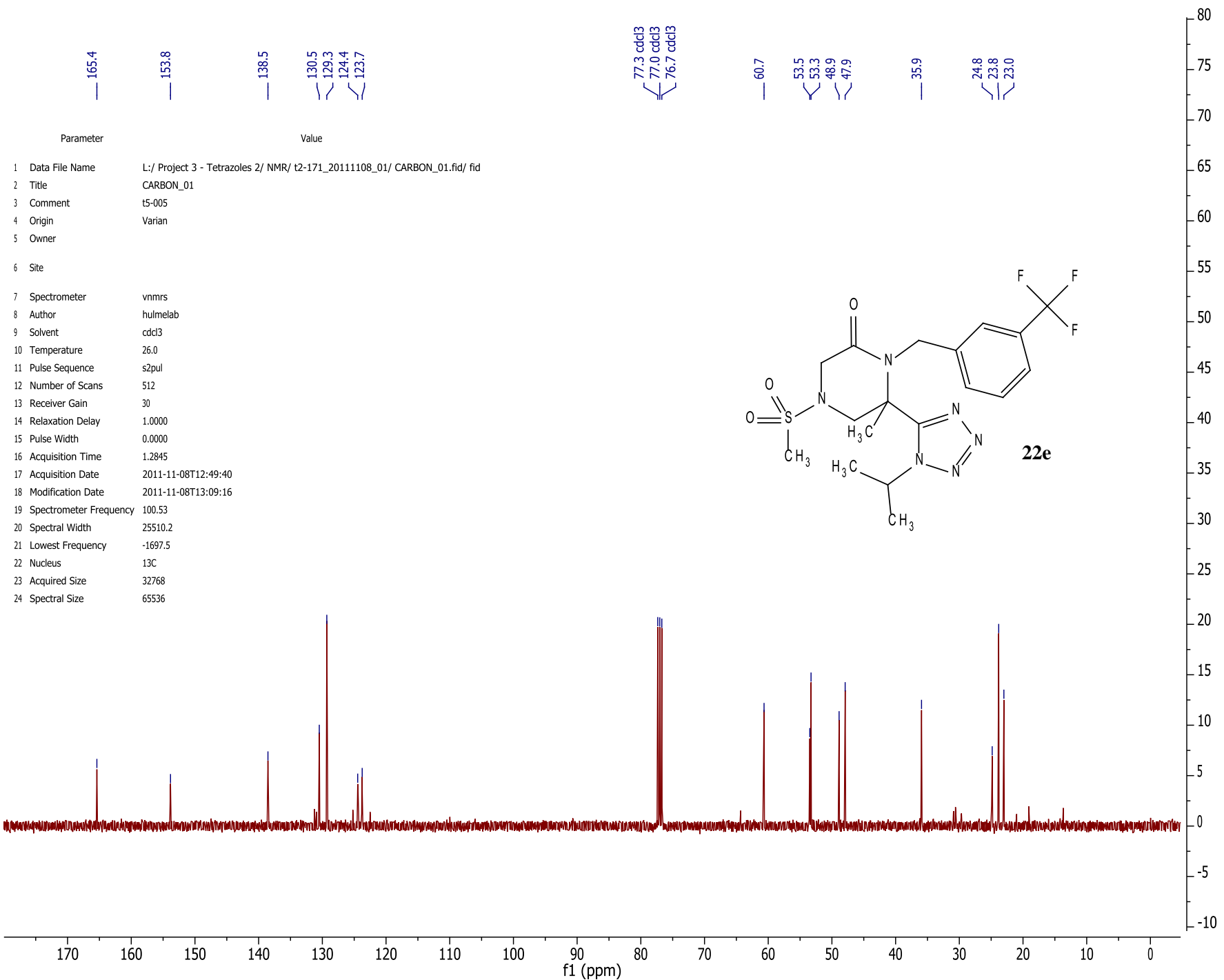


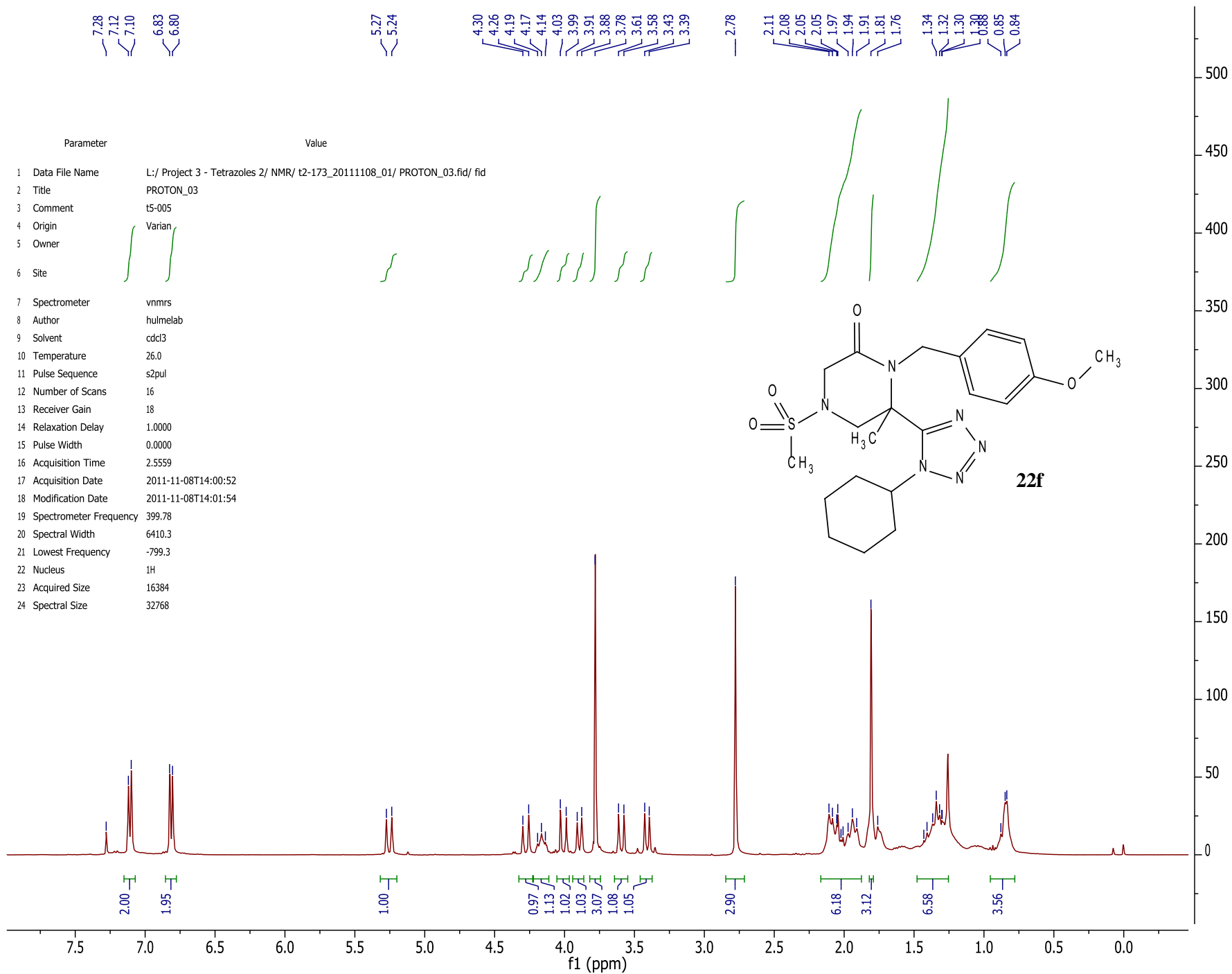


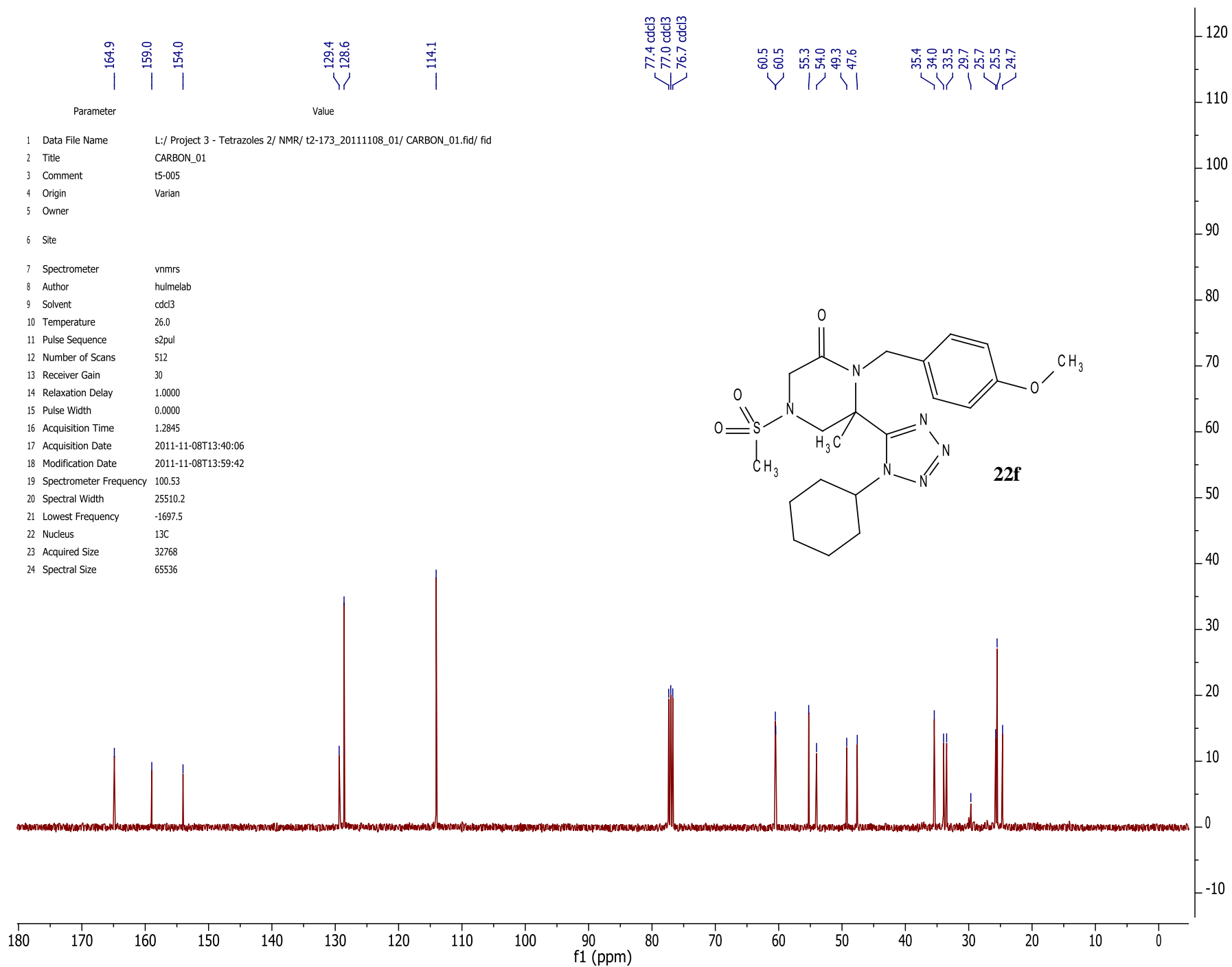


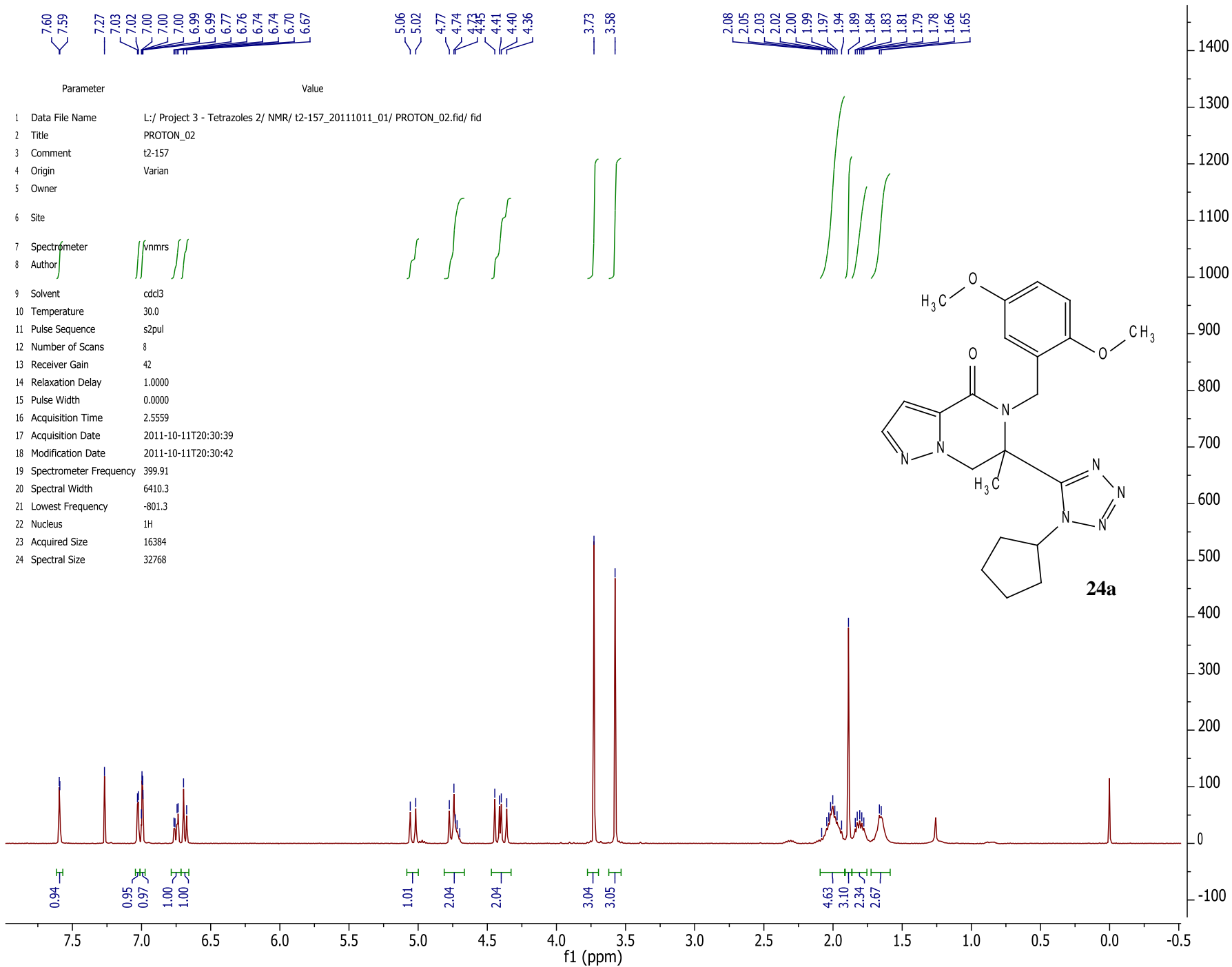


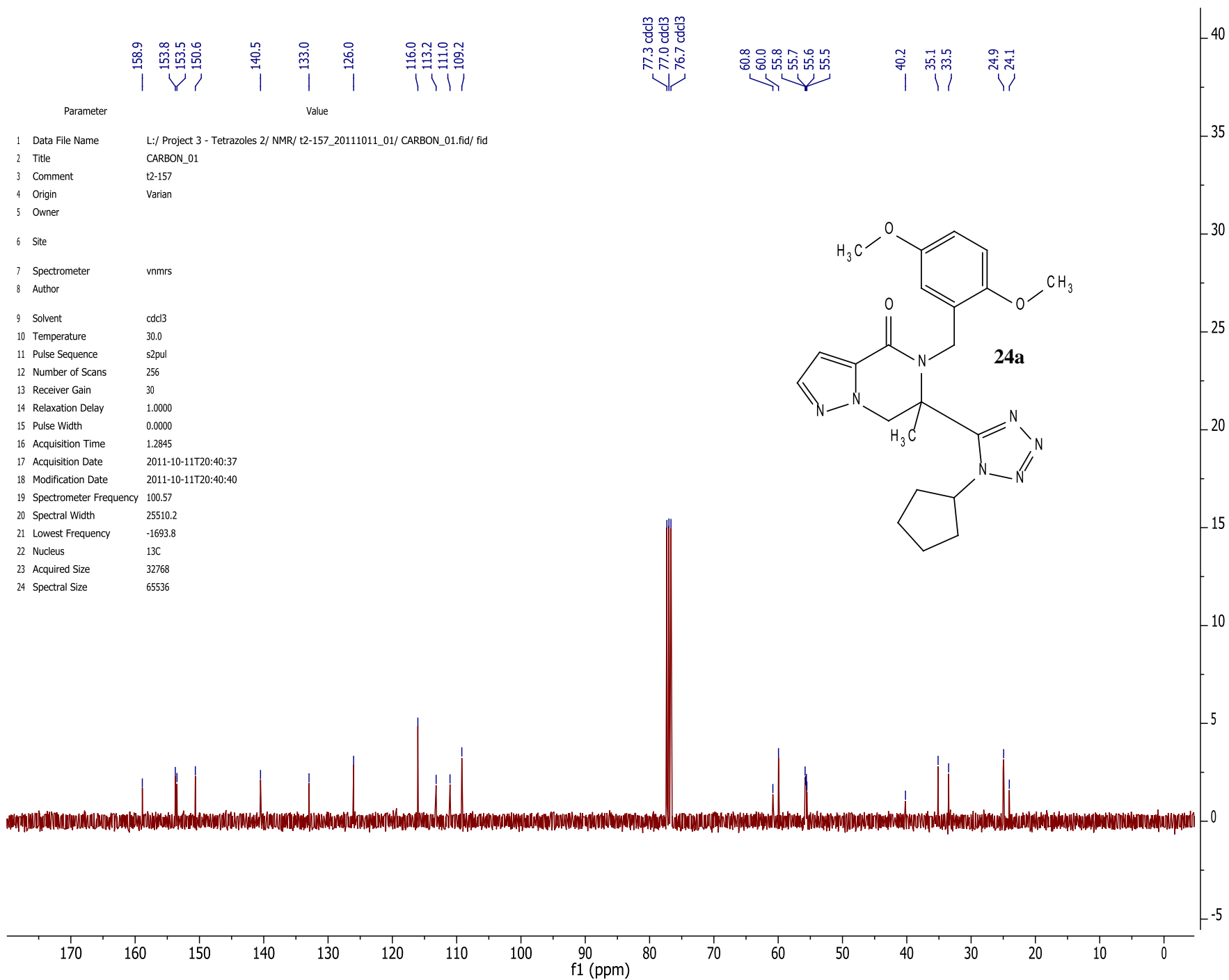


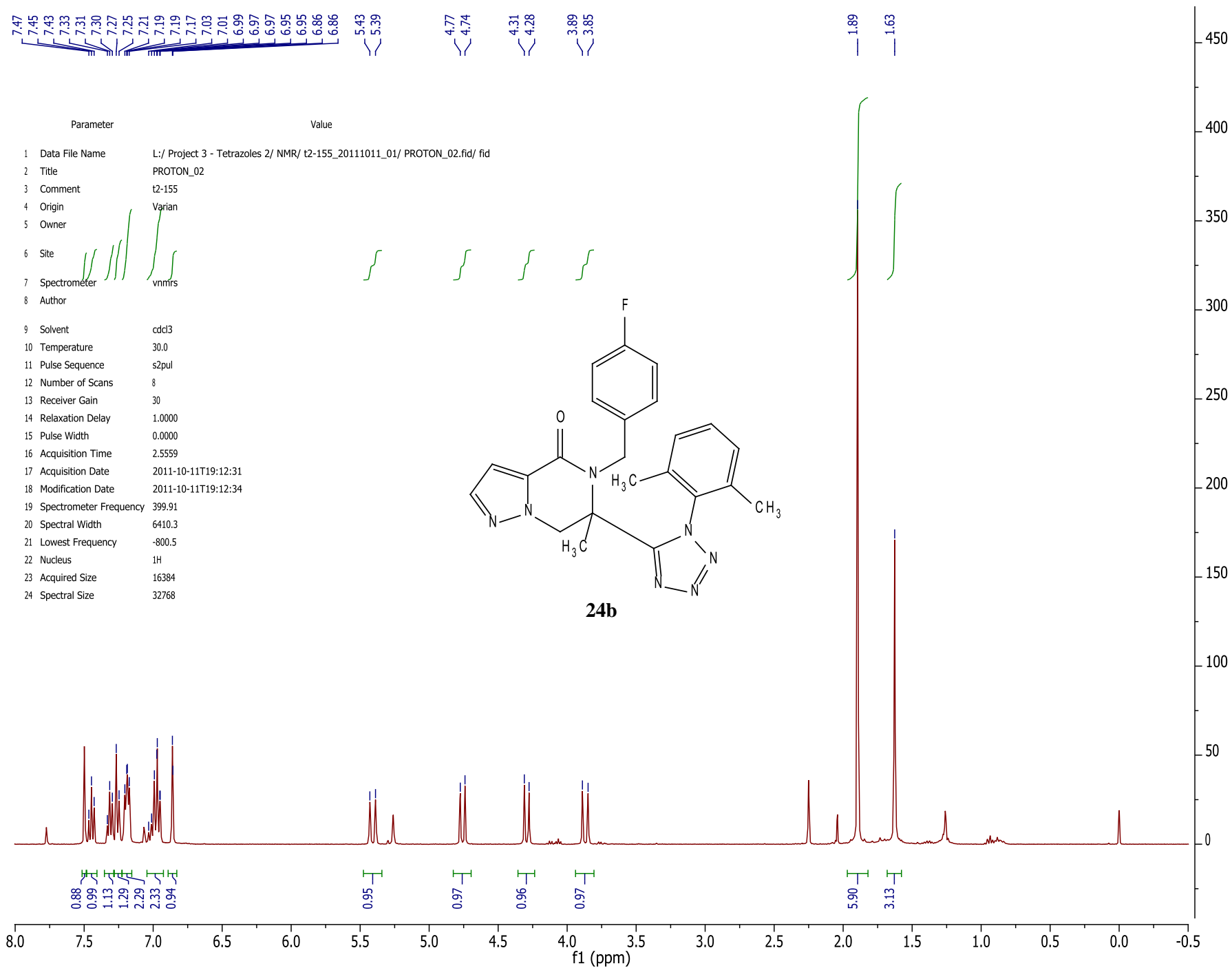




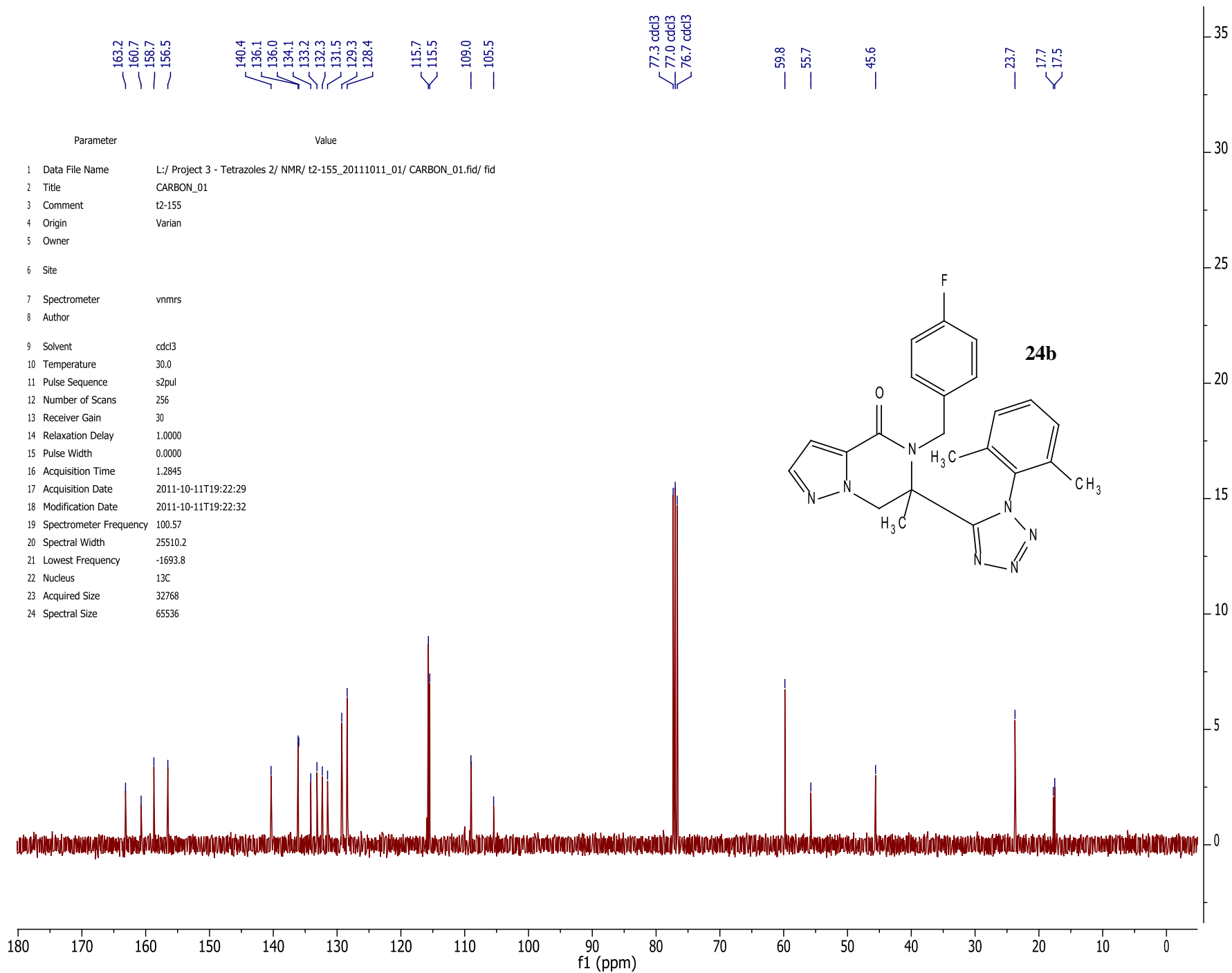


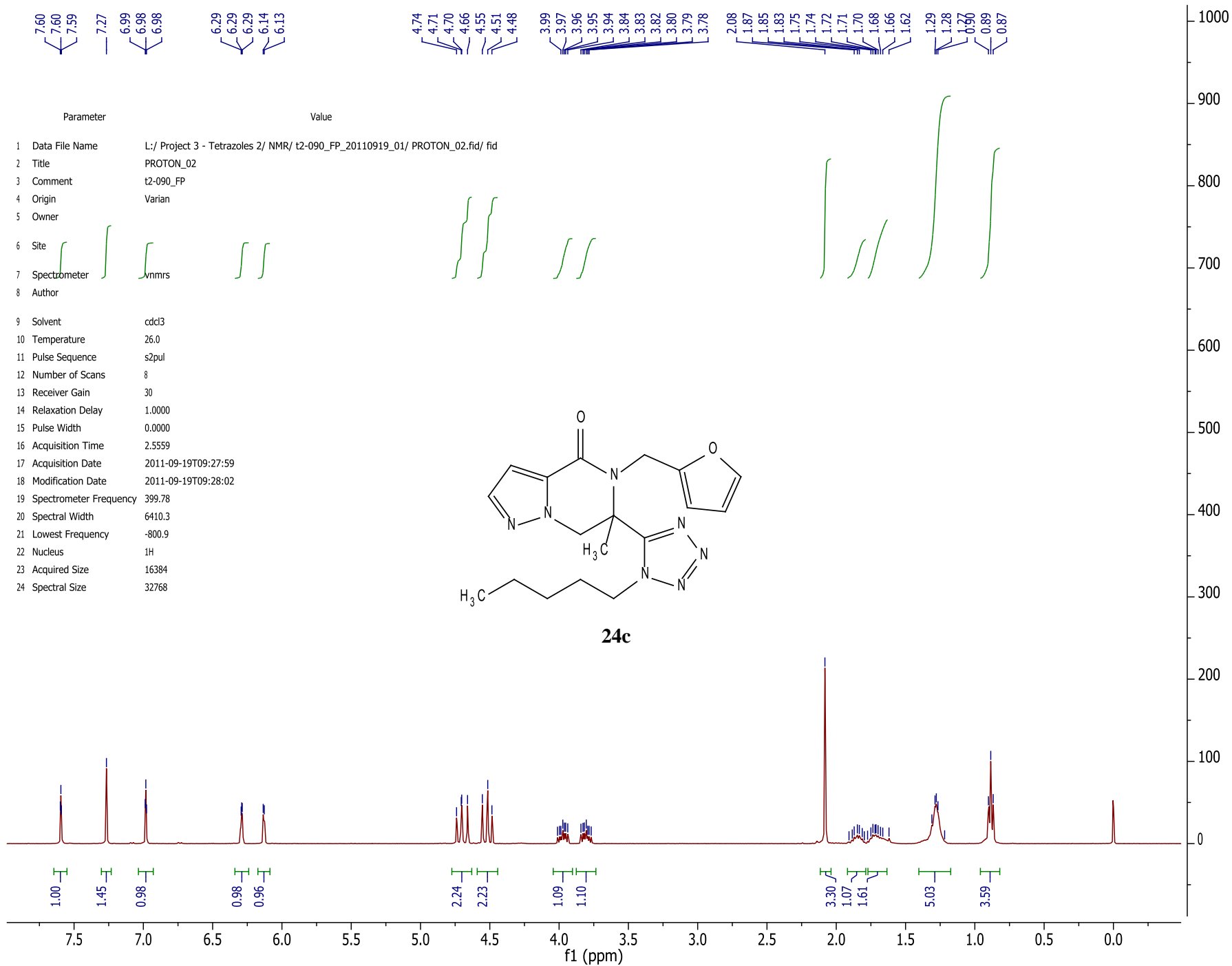


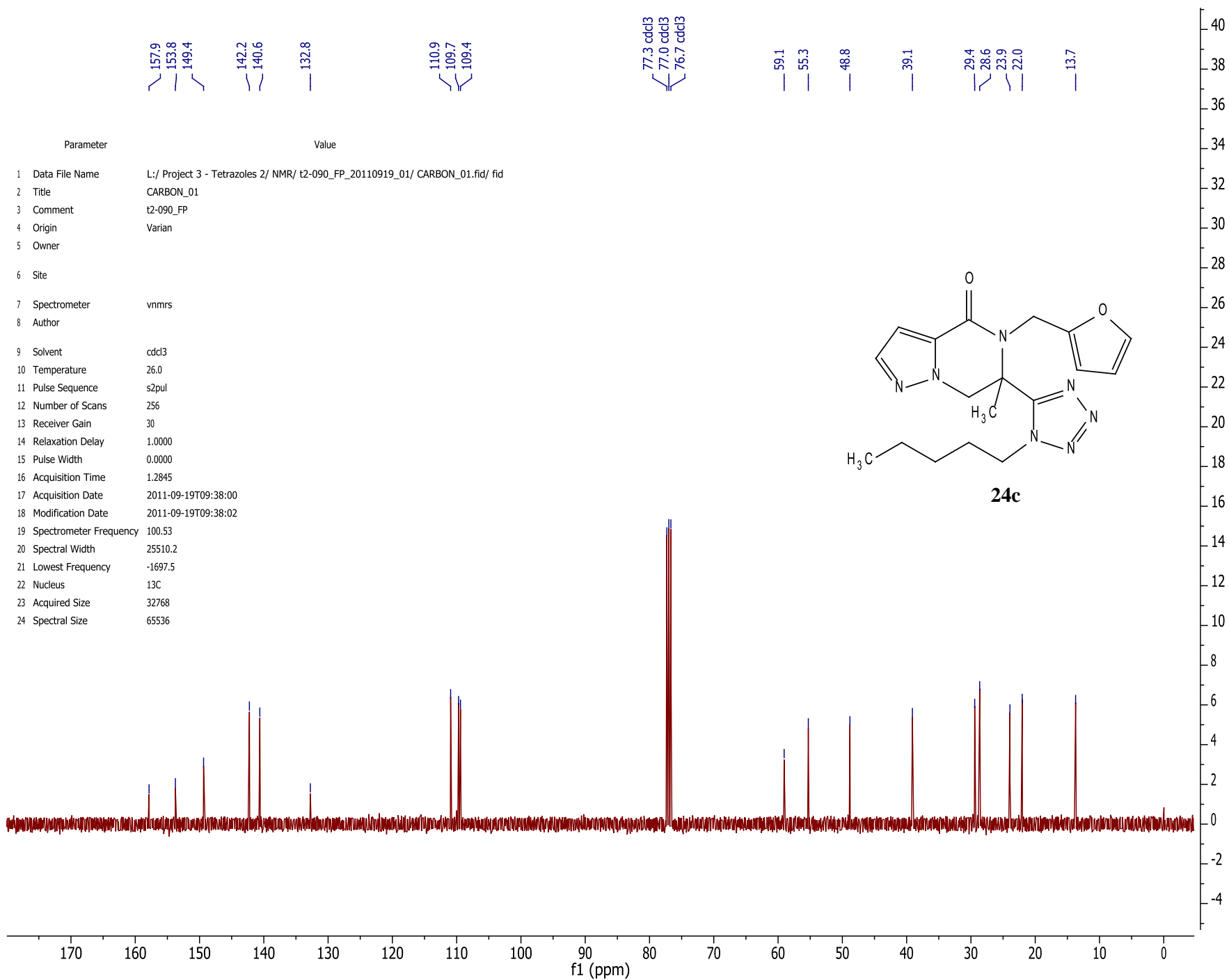




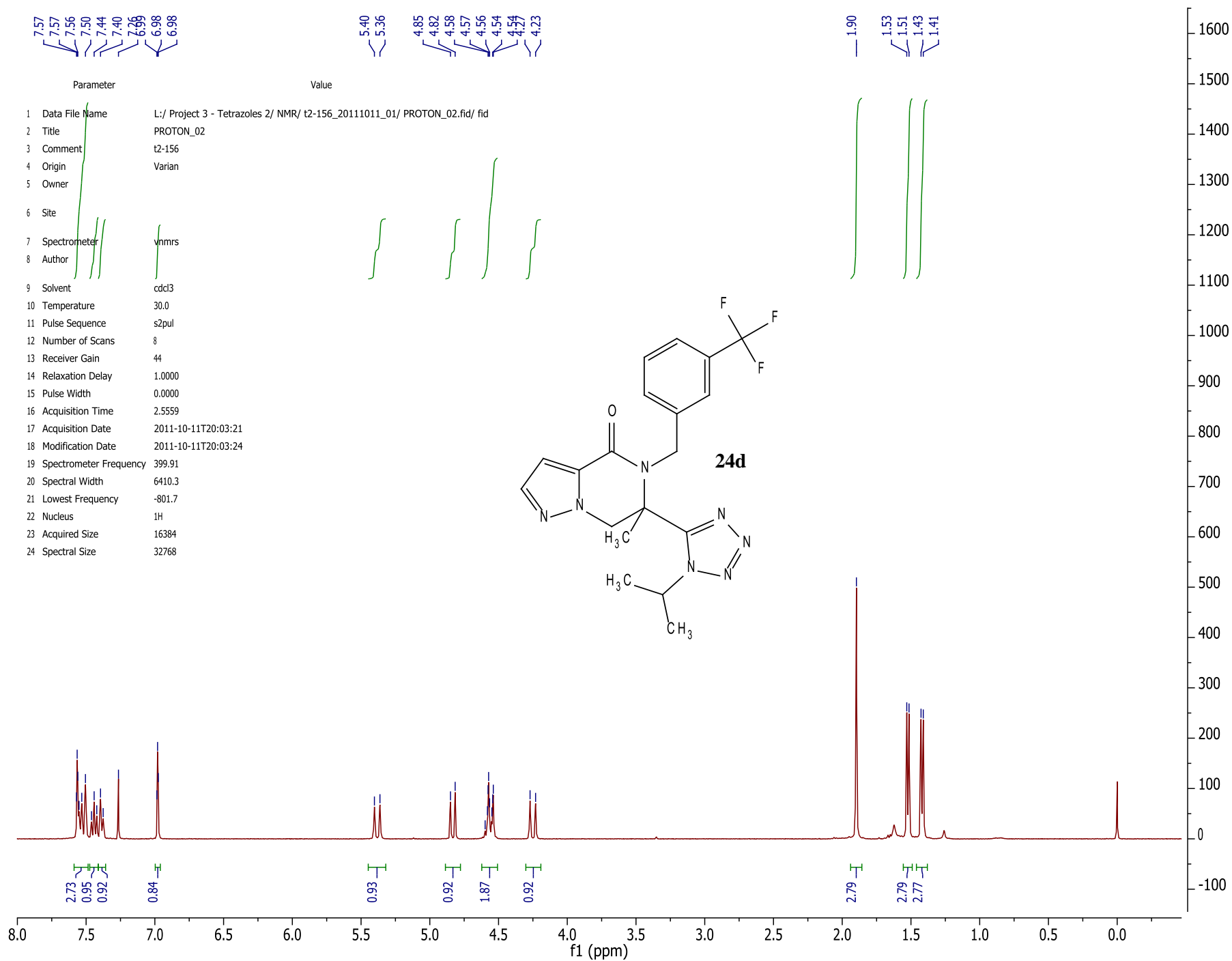
Parameter	Value
1 Data File Name	L:/ Project 3 - Tetrazoles 2/ NMR/ t2-155_20111011_01/ PROTON_02.fid/ fid
2 Title	PROTON_02
3 Comment	t2-155
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	nmr5
8 Author	
9 Solvent	cdcl3
10 Temperature	30.0
11 Pulse Sequence	s2pul
12 Number of Scans	8
13 Receiver Gain	30
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	2.5559
17 Acquisition Date	2011-10-11T19:12:31
18 Modification Date	2011-10-11T19:12:34
19 Spectrometer Frequency	399.91
20 Spectral Width	6410.3
21 Lowest Frequency	-800.5
22 Nucleus	1H
23 Acquired Size	16384
24 Spectral Size	32768

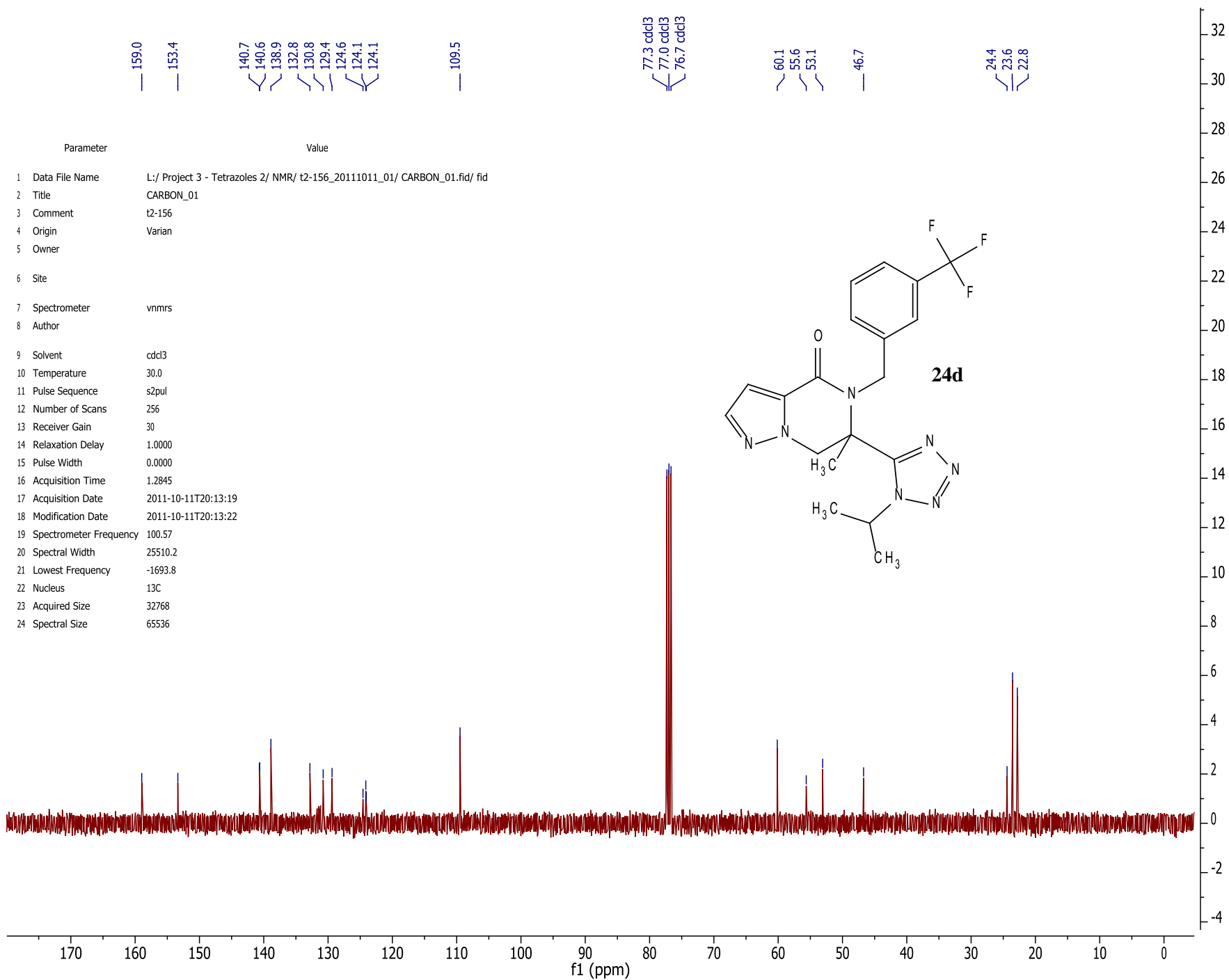


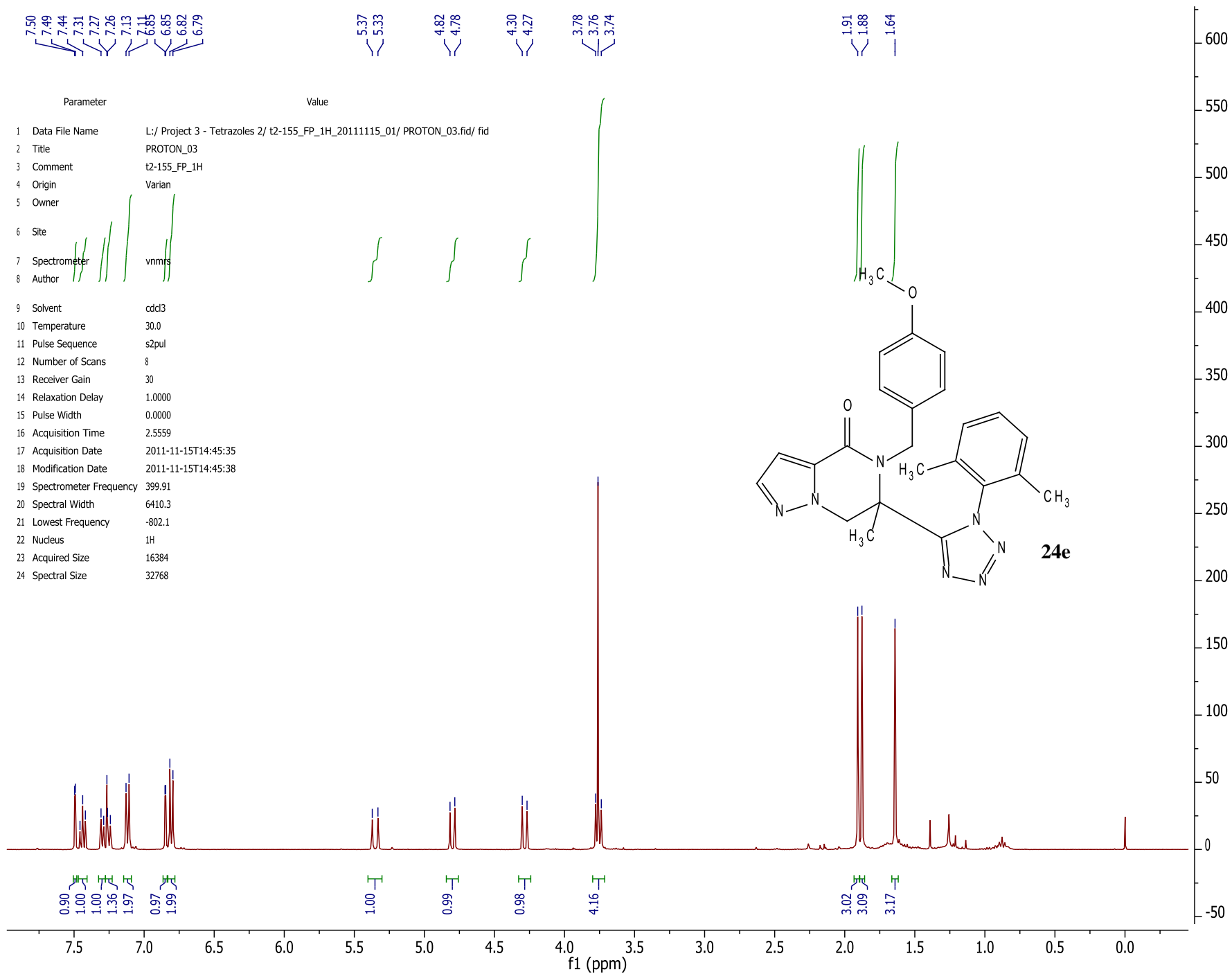


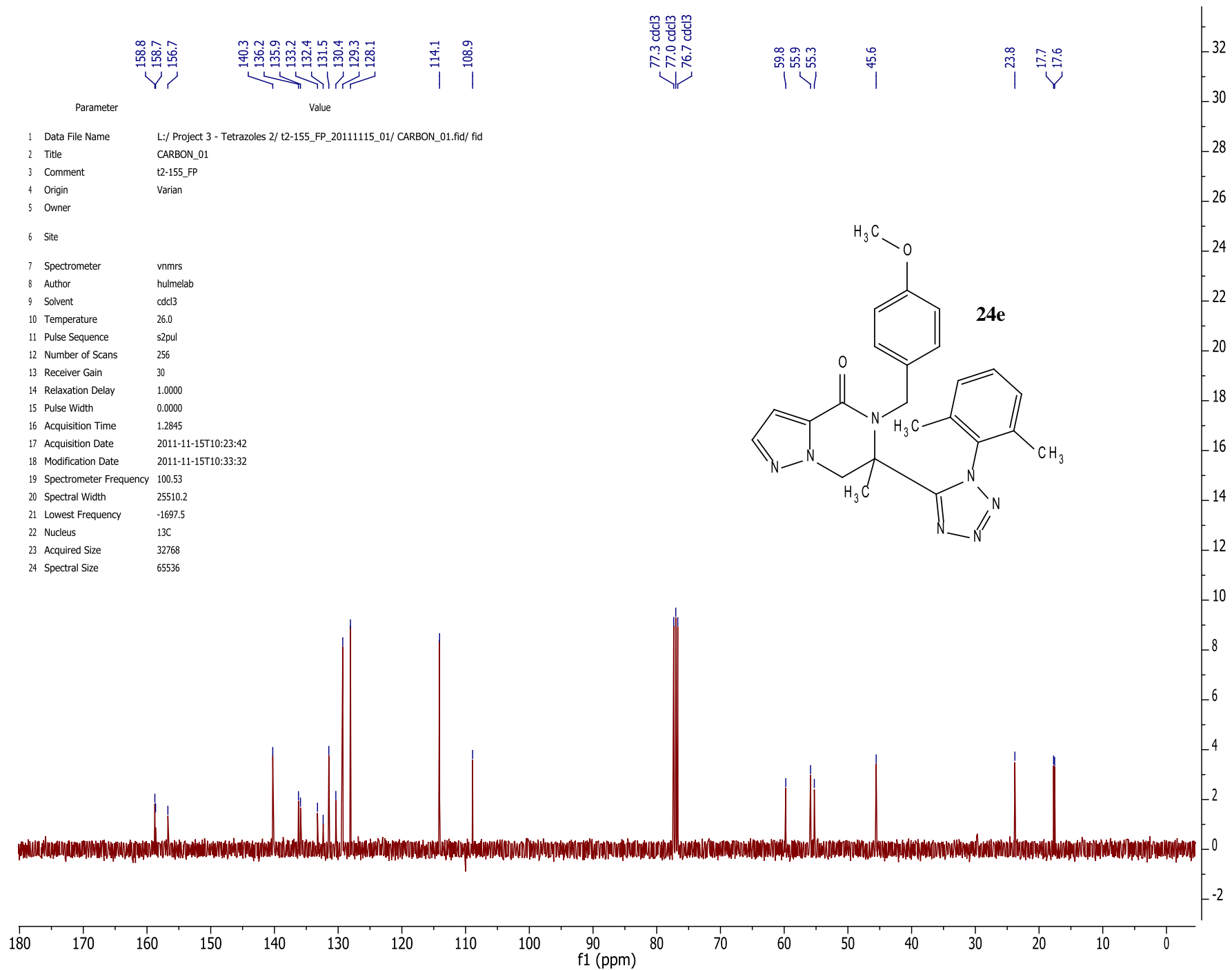


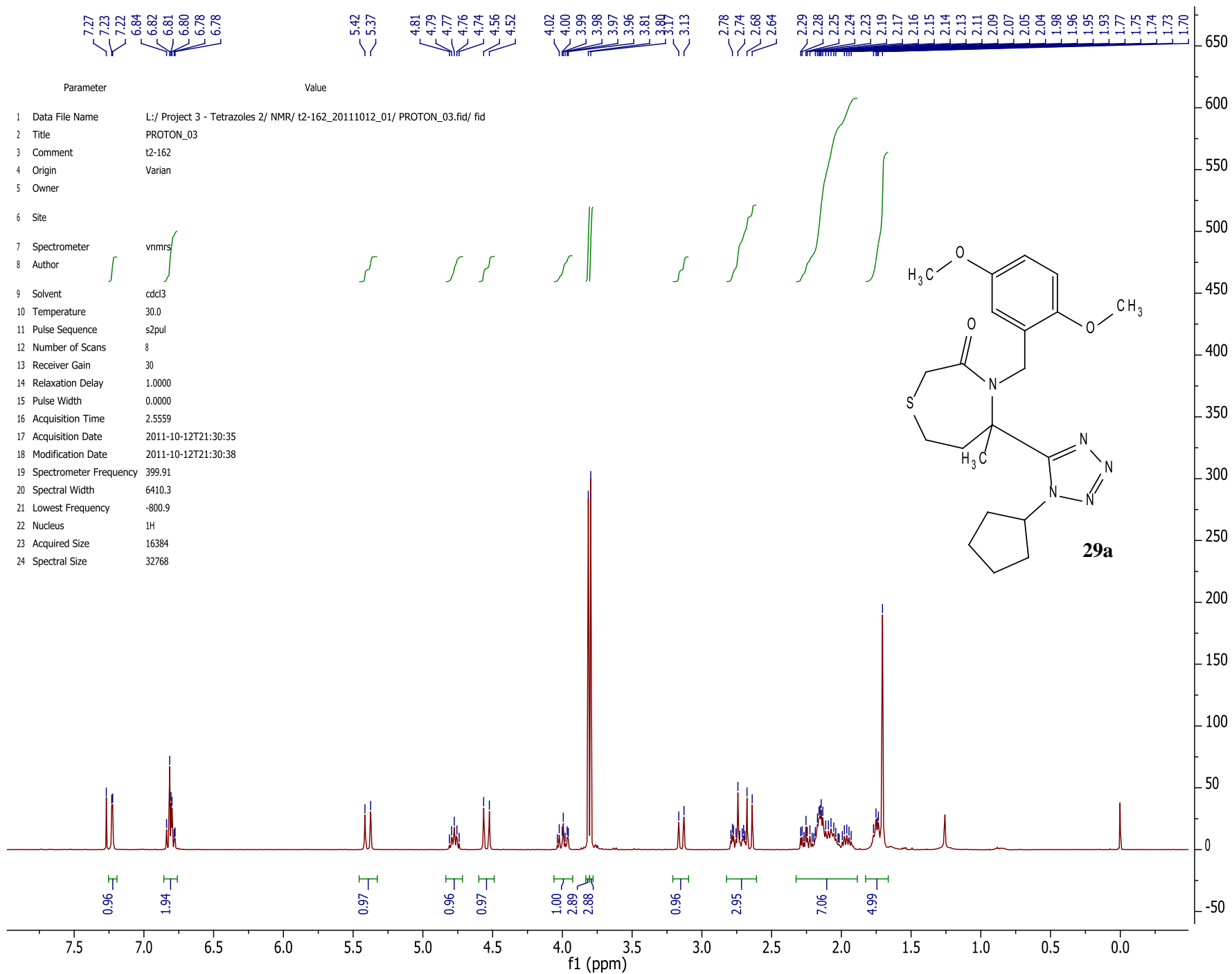
Parameter	Value
1 Data File Name	L:/ Project 3 - Tetrazoles 2/ NMR/ t2-090_FP_20110919_01/ CARBON_01.fid/ fid
2 Title	CARBON_01
3 Comment	t2-090_FP
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	nmrs
8 Author	
9 Solvent	cdcl3
10 Temperature	26.0
11 Pulse Sequence	s2pul
12 Number of Scans	256
13 Receiver Gain	30
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.2845
17 Acquisition Date	2011-09-19T09:38:00
18 Modification Date	2011-09-19T09:38:02
19 Spectrometer Frequency	100.53
20 Spectral Width	25510.2
21 Lowest Frequency	-1697.5
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

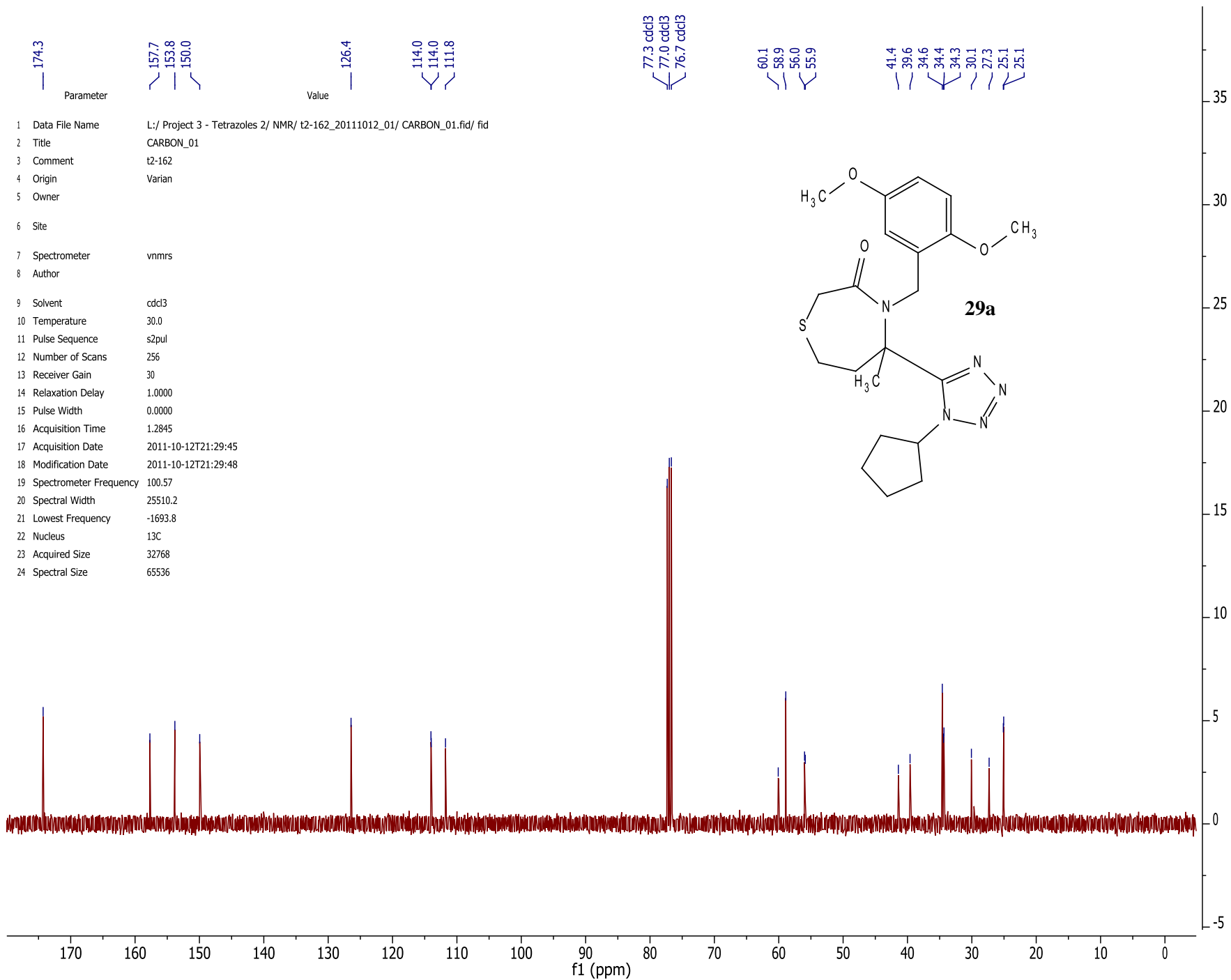


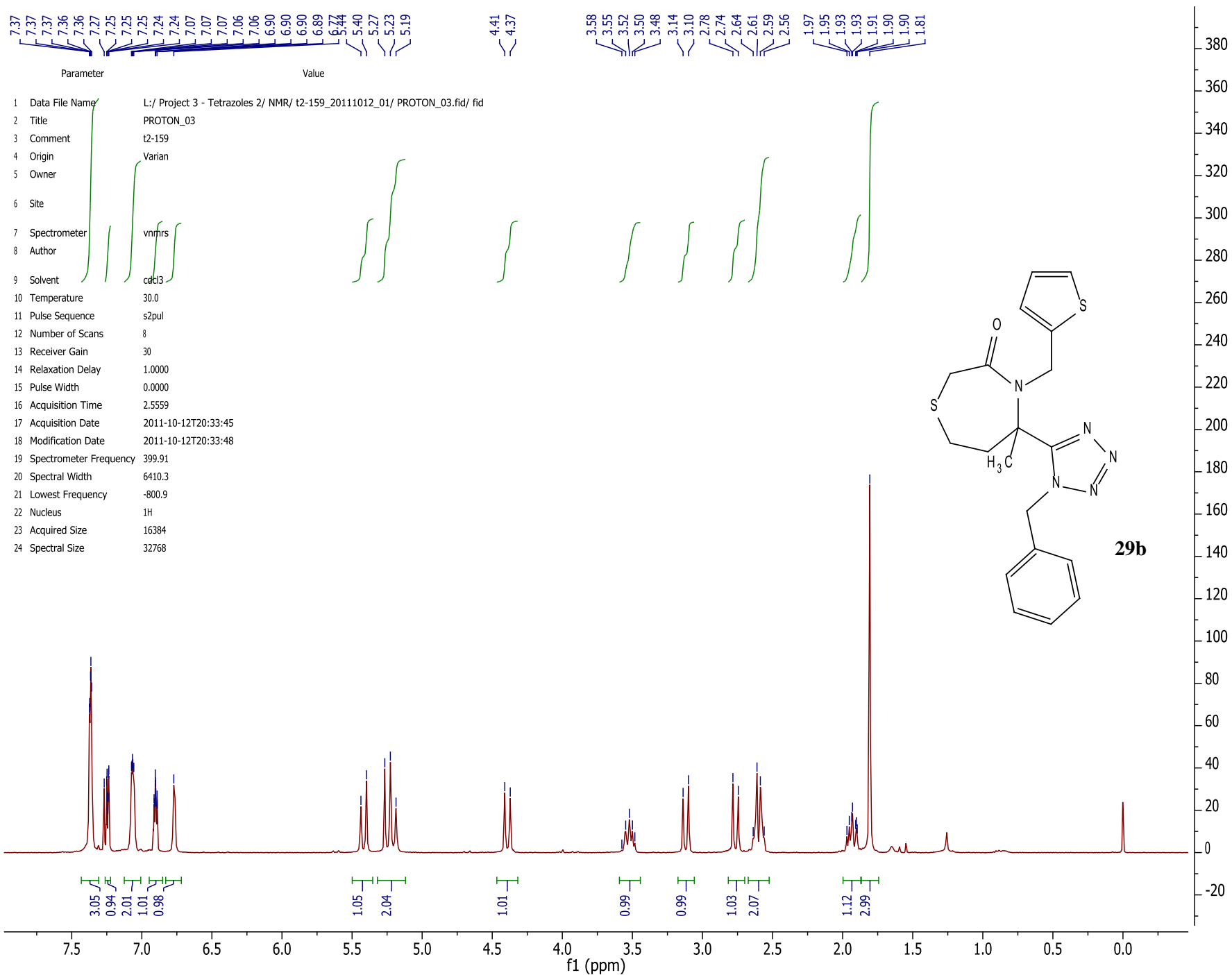












Parameter Value

1 Data File Name L:/ Project 3 - Tetrazoles 2/ NMR/ t2-159_20111012_01/ PROTON_03.fid/ fid

2 Title PROTON_03

3 Comment t2-159

4 Origin Varian

5 Owner

6 Site

7 Spectrometer vnmr5

8 Author

9 Solvent cdcl3

10 Temperature 30.0

11 Pulse Sequence s2pul

12 Number of Scans 8

13 Receiver Gain 30

14 Relaxation Delay 1.0000

15 Pulse Width 0.0000

16 Acquisition Time 2.5559

17 Acquisition Date 2011-10-12T20:33:45

18 Modification Date 2011-10-12T20:33:48

19 Spectrometer Frequency 399.91

20 Spectral Width 6410.3

21 Lowest Frequency -800.9

22 Nucleus 1H

23 Acquired Size 16384

24 Spectral Size 32768

