

Supplementary data for article:

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Electronic Supplementary material for:

Aqueous Synthesis of *N,S*-Dialkylthiophosphoramides: Design, Optimisation and Application to Library Construction and Anti-Leishmanial Testing

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Kinetic studies on the decomposition of ethanolamine thiophosphoroamidate

Disappearance of the thiophosphoroamidate

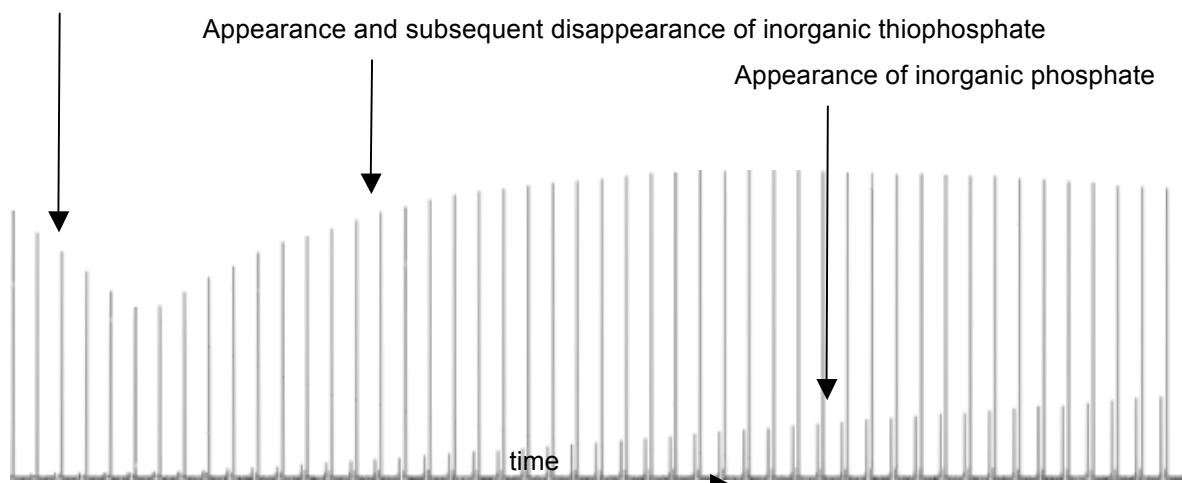


Figure 1. Time-resolved ^{31}P NMR spectra for the decomposition of ethanolamine thiophosphoramide at $\text{pD} \sim 2.6$ (citrate). The figure shows horizontally compressed spectra taken at time points increasing from the left to the right.

The intensities of the peaks corresponding to the thiophosphoroamidate, normalised with the highest intensity peak in the spectra, set to have the value 1, were plotted as a pseudo first order function of time and least squares fittings were performed against an exponential decay curve $I_t = I_0 \times e^{-k_{\text{obs}} t}$. An example of the data and its fitting are shown below.

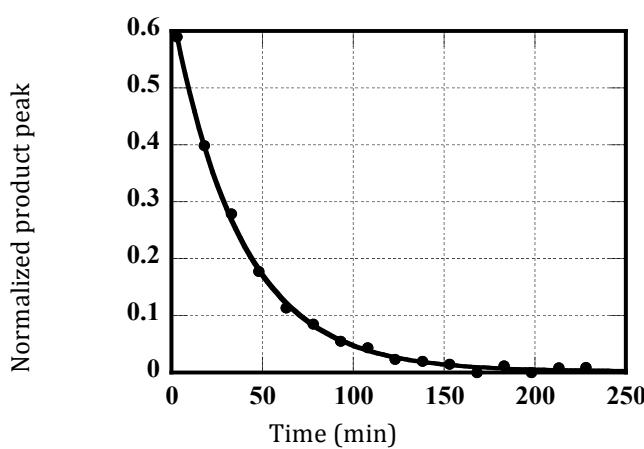


Figure 2: An example of thiophosphoroamidate degradation followed by ^{31}P NMR

The recorded pD of the analysed solution was then expressed as $\text{pH} \pm 10\%$ ($\text{pH} = \text{pD} - 0.4$) and plotted against k_{obs} for the corresponding buffer (ESI table 1, main manuscript figure 3).

Table 2: Observed kinetic data for the aqueous ethanolamine thiophosphoroamidate kinetic studies. In the experiments with inconstant pH (0.5 M buffer), pH was represented as the interval from the start to the end of experiment

pH (buffer)	4 M buffer	0.5 M buffer
	$k_o \times 10^4$ (s ⁻¹),	$k_o \times 10^4$ (s ⁻¹),
10.2 (CAPS)	0.035	0.013
9.5-9.3 (CHES)	n.d.	0.22
9.2 (CHES)	0.2	n.d.
8.5-9.2 (EPPS)	n.d.	0.42
8.7 (EPPS)	0.38	n.d.
7.9 (TRIS)	0.77	n.d.
7.4-7.7 (TRIS)	n.d.	2.7
7.5 (HEPES)	n.d.	3.2
7.4 (TRIS)	1.3	n.d.
7.1 (HEPES)	2.3	n.d.
6.9-7.1 (MES)	n.d.	5.5
6.8 (MES)	4.5	n.d.
5.7-6.2 (Acetate)	n.d.	5.8
5.8 (MES)	5.0	n.d.
5.3 (Acetate)	4.5	n.d.
5 (Acetate)	3.8	n.d.
3.6 (Citrate)	4.7	n.d.
2.9 (Citrate)	2.5	n.d.
2.2 (Citrate)	3.8	n.d.

N-thiophosphorylation of simple hydrophobic amines and S-alkylation of the resulting N-thiophosphoramidate anions during.

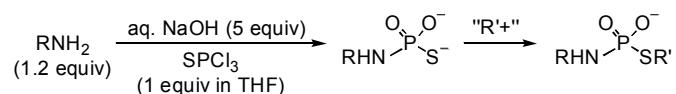
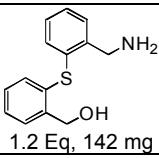
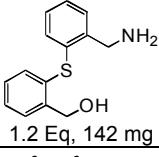
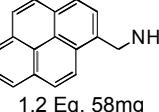
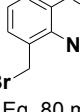
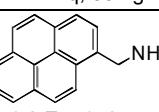
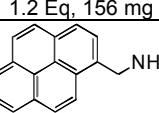
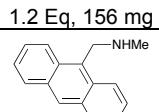
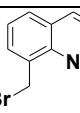
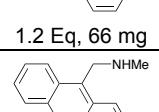
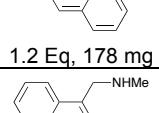
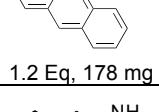
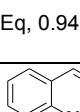
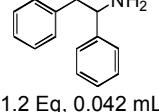
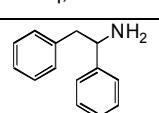
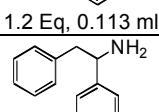
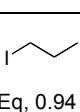
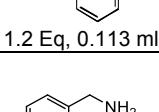
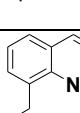
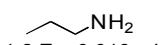
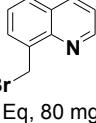
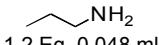
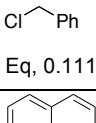
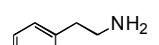
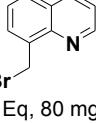
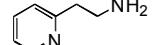
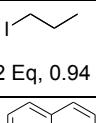
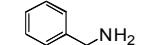
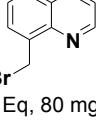
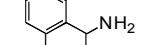
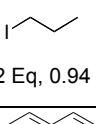
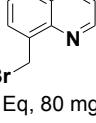
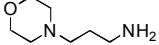
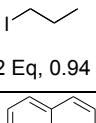
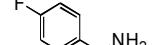
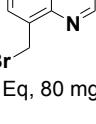
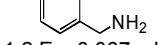
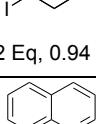
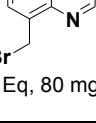


Table 3: Quantities employed during the syntheses of these species are summarized below.

Entry number in Table 2 in main manuscript	RNH ₂	Alkylation agent	Additional 1 M NaOH (mL) added during alkylation step
20a	 1.2 Eq, 0.031 mL	 2 Eq, 80 mg	0
20b	 1.2 Eq, 0.083 mL	ClCH ₂ Ph 2 Eq, 0.111 mL	0
20c	 1.2 Eq, 0.083 mL	I-CH ₂ -CH ₂ 2 Eq, 0.94 mL	0
21a	 1.2 Eq, 39 mg	 2 Eq, 80 mg	0.09
21b	 1.2 Eq, 105 mg	ClCH ₂ Ph 2 Eq, 0.111 mL	0
21c	 1.2 Eq, 105 mg	I-CH ₂ -CH ₂ 2 Eq, 0.94 mL	0
22a	 1.2 Eq, 0.031 mL	 2 Eq, 80 mg	0.09
22b	 1.2 Eq, 0.083 mL	ClCH ₂ Ph 2 Eq, 0.111 mL	0
22c	 1.2 Eq, 0.083 mL	I-CH ₂ -CH ₂ 2 Eq, 0.94 mL	0
23a	 1.2 Eq, 53 mg	 2 Eq, 80 mg	0.198

23b	 1.2 Eq, 142 mg	 2 Eq, 0.111 ml	0.2
23c	 1.2 Eq, 142 mg	 2 Eq, 0.94 ml	0.2
24a	 1.2 Eq, 58 mg	 2 Eq, 80 mg	0
24b	 1.2 Eq, 156 mg	 2 Eq, 0.111 ml	0.2
24c	 1.2 Eq, 156 mg	 2 Eq, 0.94 ml	0.2
25a	 1.2 Eq, 66 mg	 2 Eq, 80 mg	0.198
25b	 1.2 Eq, 178 mg	 2 Eq, 0.111 ml	0
25c	 1.2 Eq, 178 mg	 2 Eq, 0.94 ml	0
26a	 1.2 Eq, 0.042 mL	 2 Eq, 80 mg	0
26b	 1.2 Eq, 0.113 ml	 2 Eq, 0.111 ml	0
26c	 1.2 Eq, 0.113 ml	 2 Eq, 0.94 ml	0
27a	 1.2 Eq, 0.023 ml	 2 Eq, 80 mg	0
28a	 1.2 Eq, 0.016 ml	 2 Eq, 80 mg	0.09

29a	 1.2 Eq, 0.018 ml	 2 Eq, 80 mg	0
29b	 1.2 Eq, 0.048 ml	 2 Eq, 0.111	0
30a	 1.2 Eq, 0.026 ml	 2 Eq, 80 mg	0
30b	 1.2 Eq, 0.07 ml	 2 Eq, 0.94	0.75
31a	 1.2 Eq, 0.031 ml	 2 Eq, 80 mg	0.198
31b	 1.2 Eq, 0.083 ml	 2 Eq, 0.94	0.75
32a	 1.2 Eq, 0.031 ml	 2 Eq, 80 mg	0
32b	 1.2 Eq, 0.83 ml	 2 Eq, 0.94	0
33a	 1.2 Eq, 0.025 ml	 2 Eq, 80 mg	0
33b	 1.2 Eq, 0.067 ml	 2 Eq, 0.94	0.75
34	none	 2 Eq, 80 mg	0

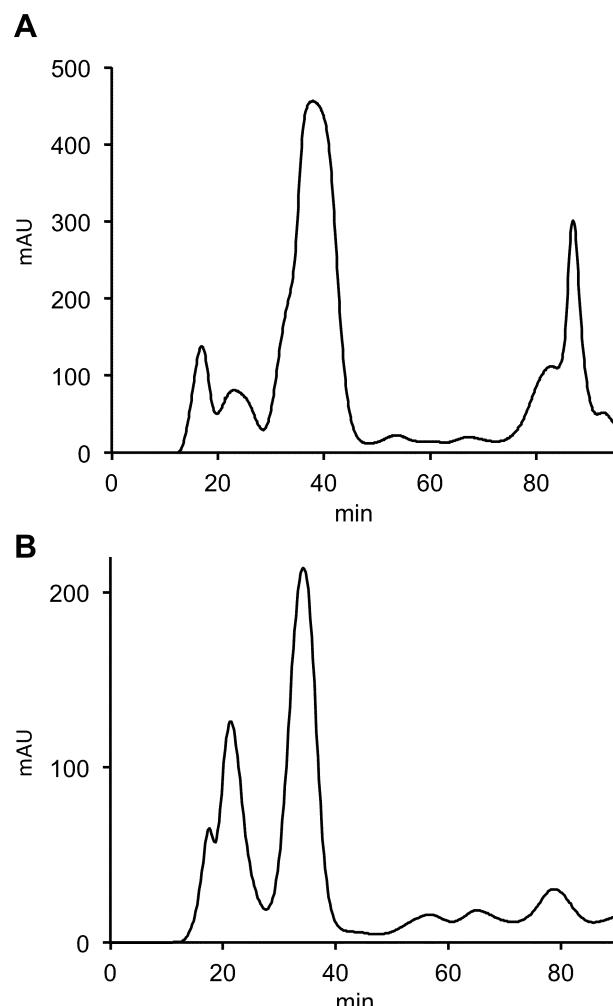


Figure 3 Chromatograms for the purification of the (A) guanosine system **12a** and (B) adenosine system **12b**. DEAE Sepharose FF media was used as the media with a gradient of triethylammonium bicarbonate (TEAB) buffer as the eluent. Absorbance was monitored at 254 nm.

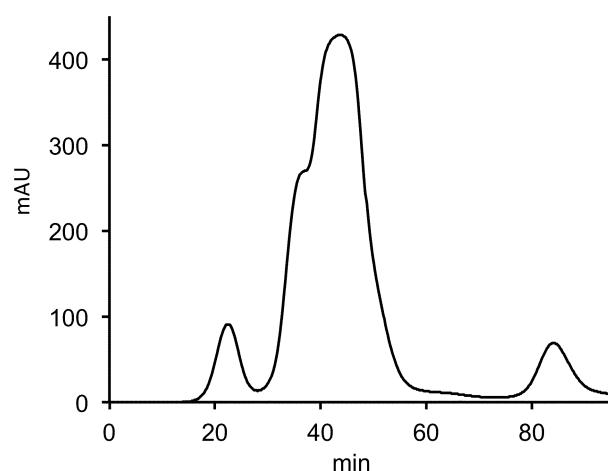
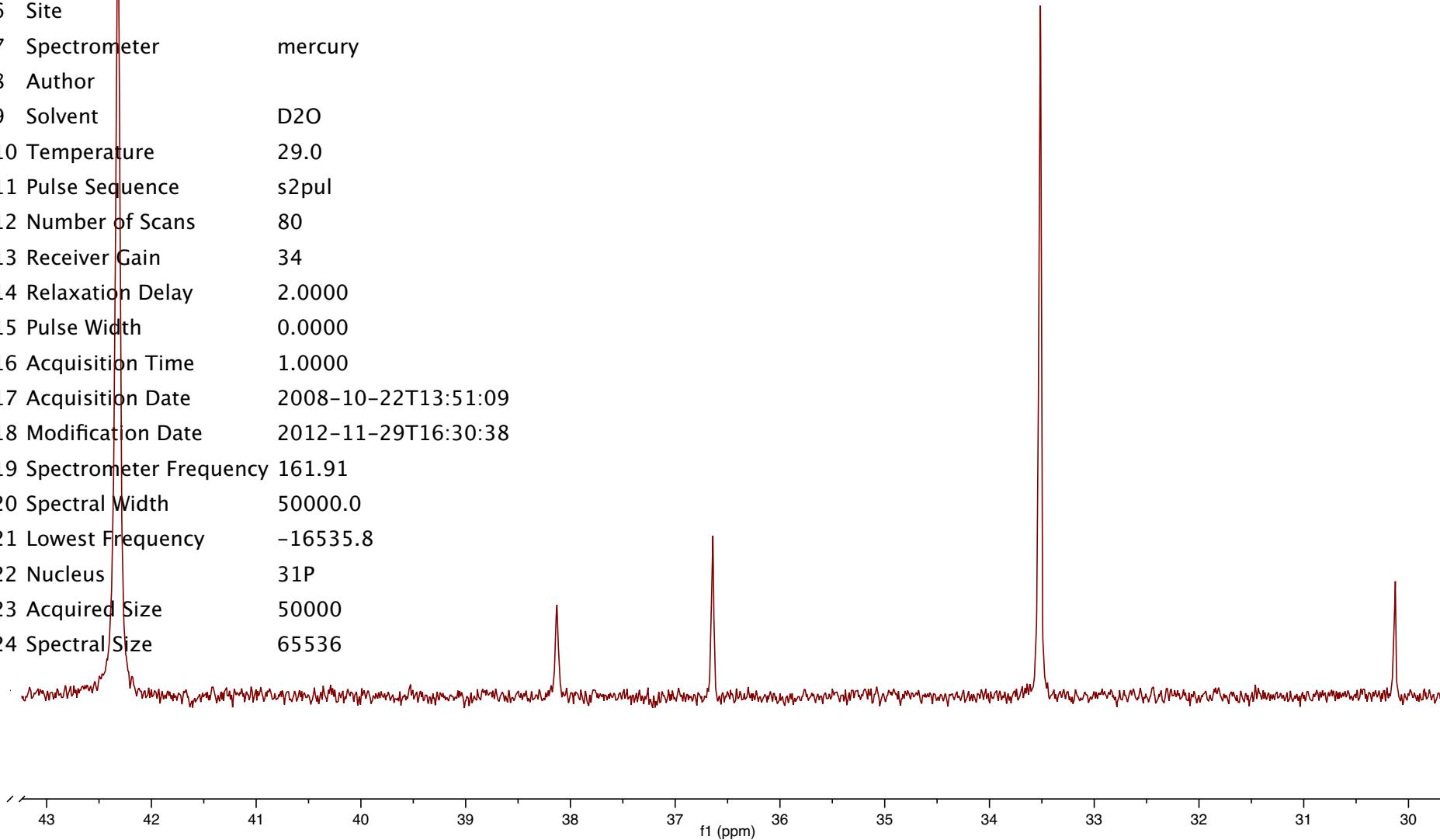
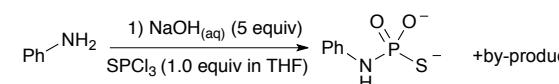
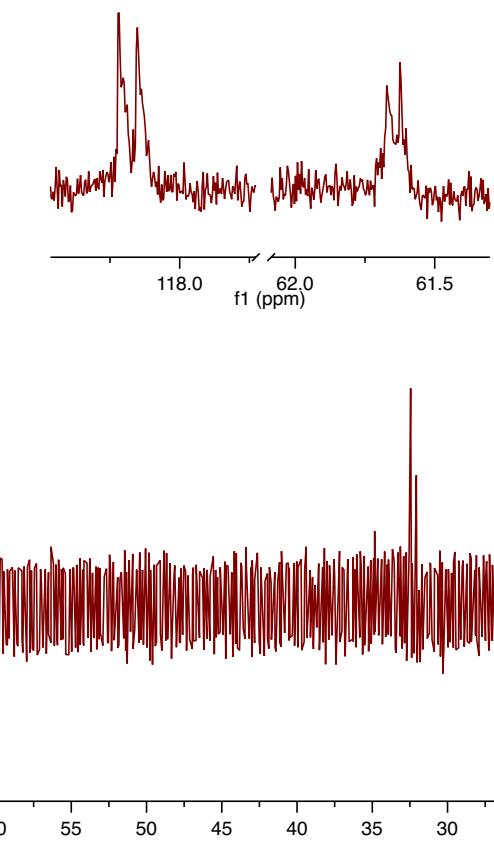
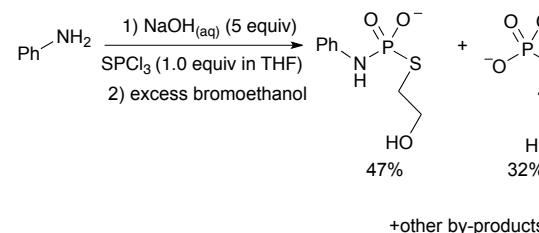


Figure 4 Ion exchange chromatography of crude benzylamine-thiophosphoryl-(5'-aminoguanosine)acetamide **16**. DEAE Sepharose FF media was used as the media with a gradient of triethylammonium bicarbonate (TEAB) buffer as the eluent. Absorbance was monitored at 254 nm.

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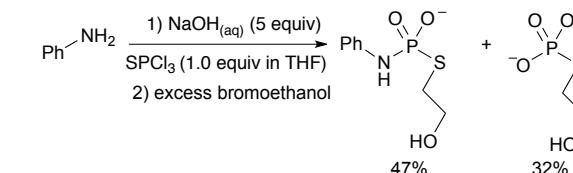
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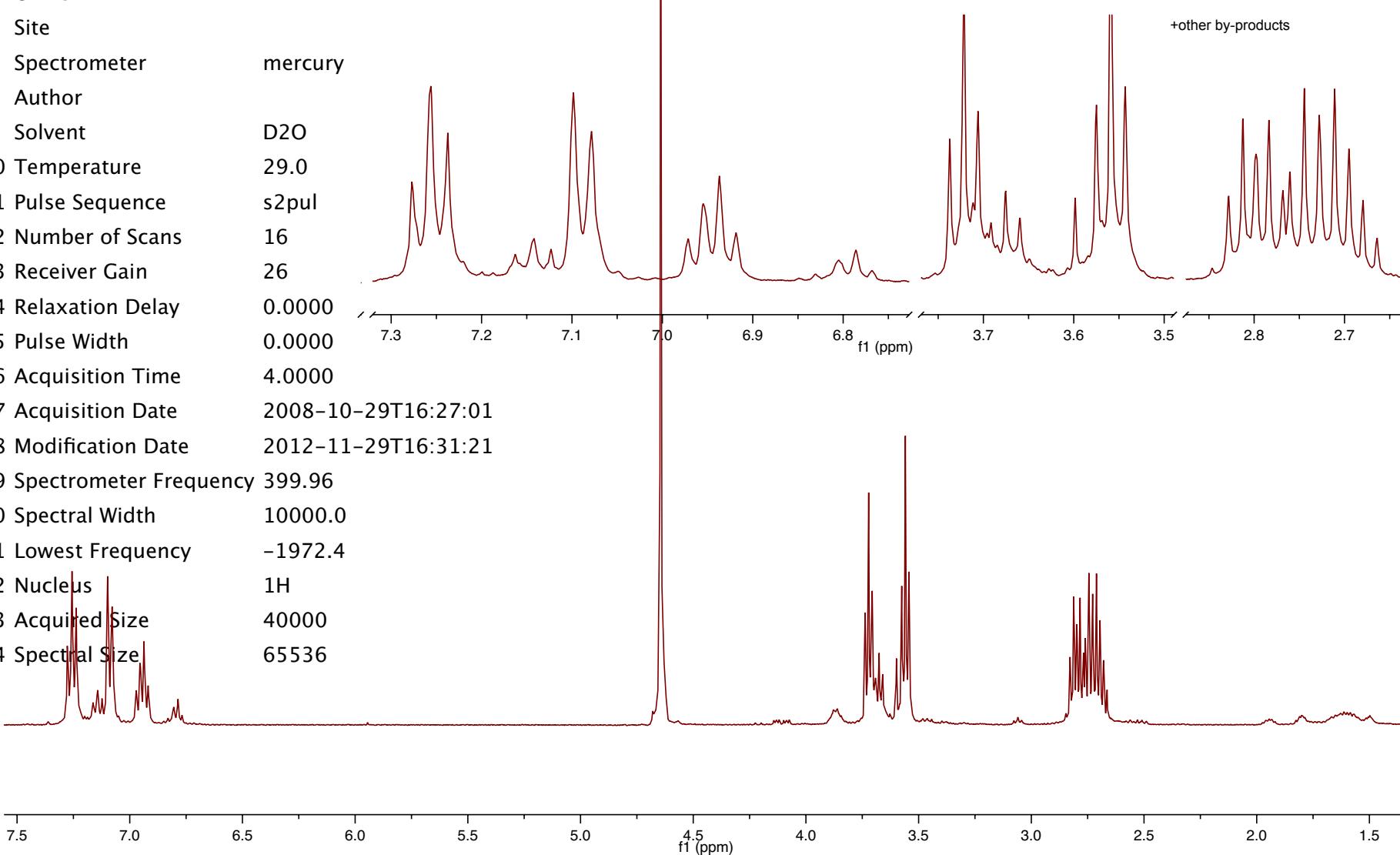
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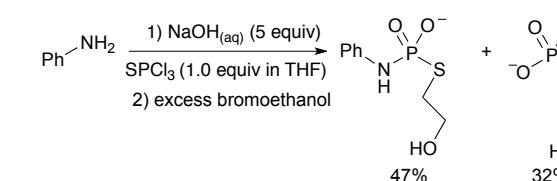
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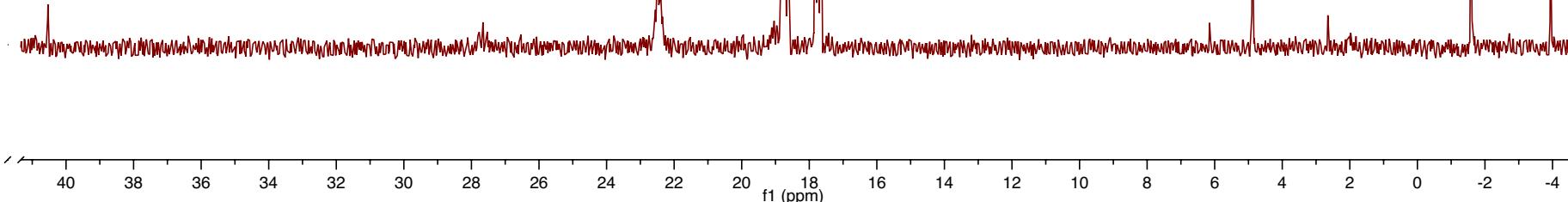
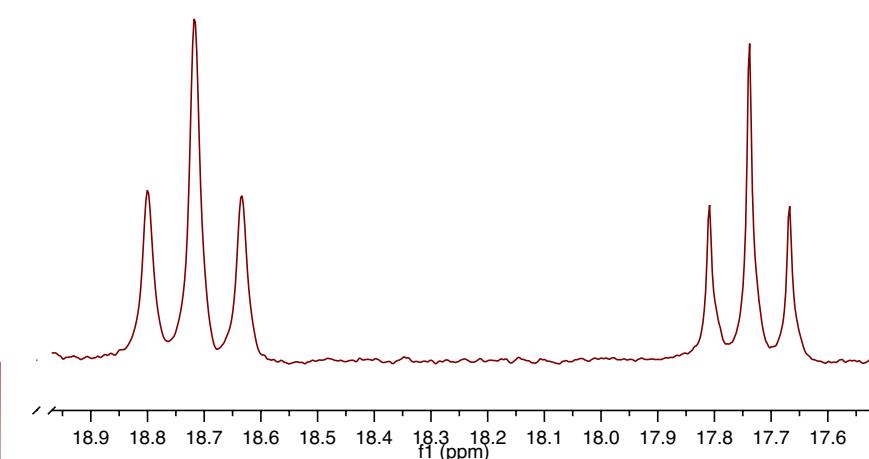
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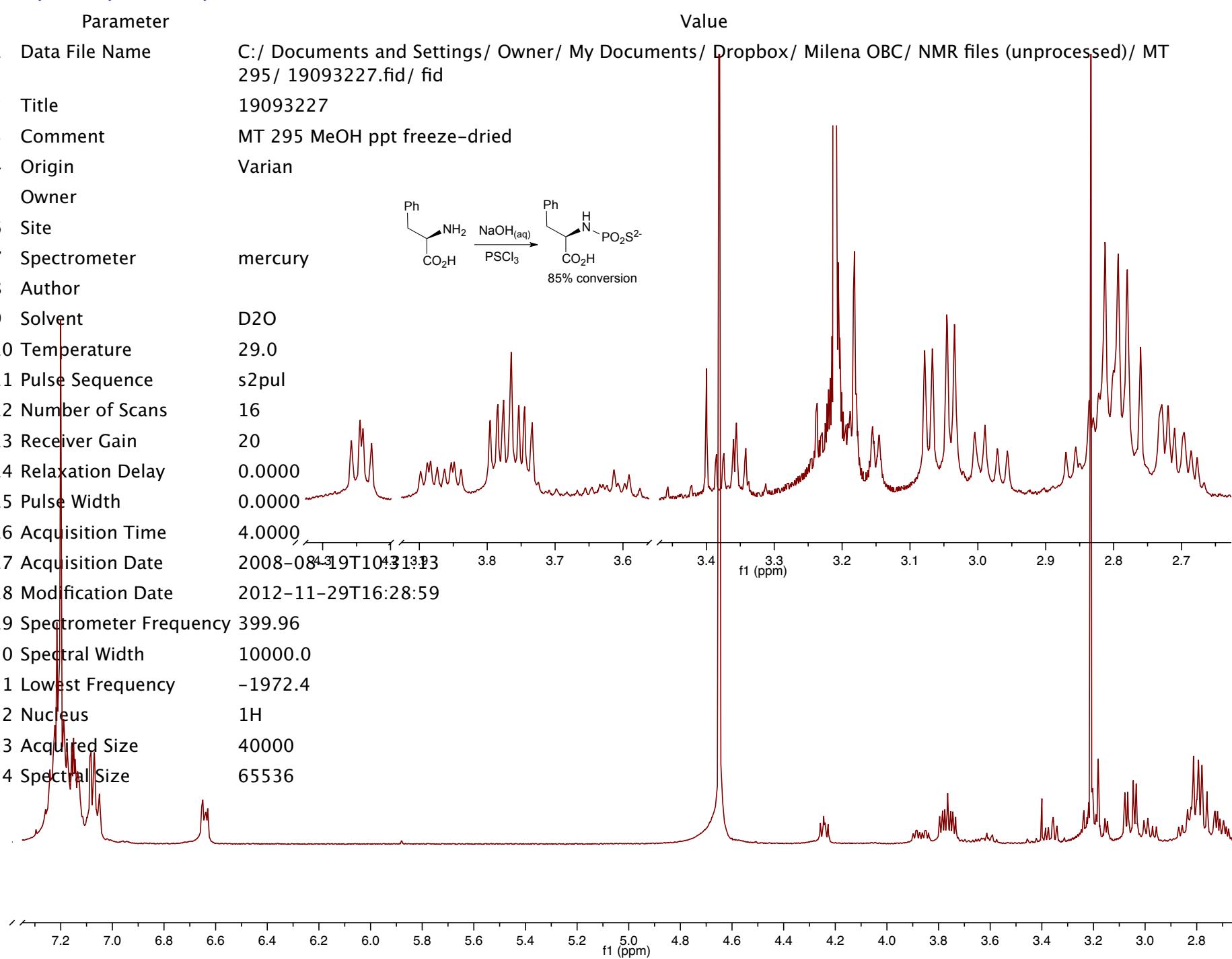
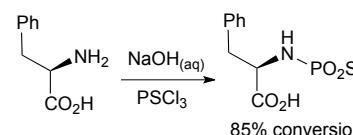
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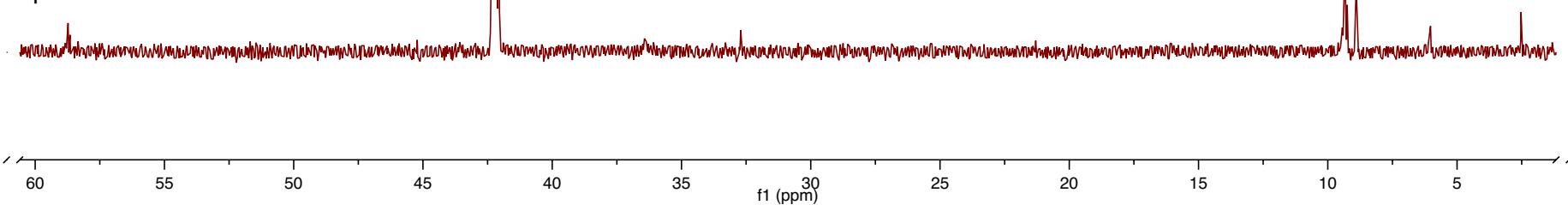
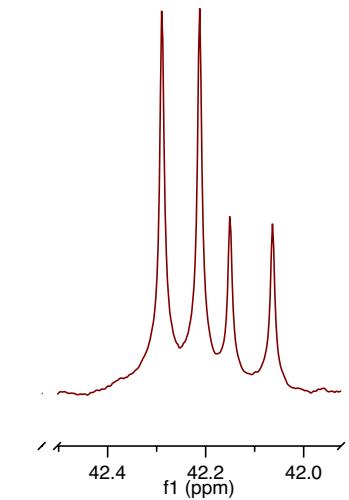
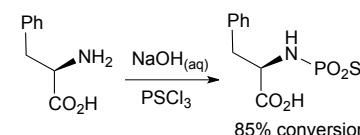
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4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	mercury
8 Author	
9 Solvent	D2O
10 Temperature	29.0
11 Pulse Sequence	s2pul
12 Number of Scans	16
13 Receiver Gain	20
14 Relaxation Delay	0.0000
15 Pulse Width	0.0000
16 Acquisition Time	4.0000
17 Acquisition Date	2008-08-19T10:43:13
18 Modification Date	2012-11-29T16:28:59
19 Spectrometer Frequency	399.96
20 Spectral Width	10000.0
21 Lowest Frequency	-1972.4
22 Nucleus	1H
23 Acquired Size	40000
24 Spectral Size	65536



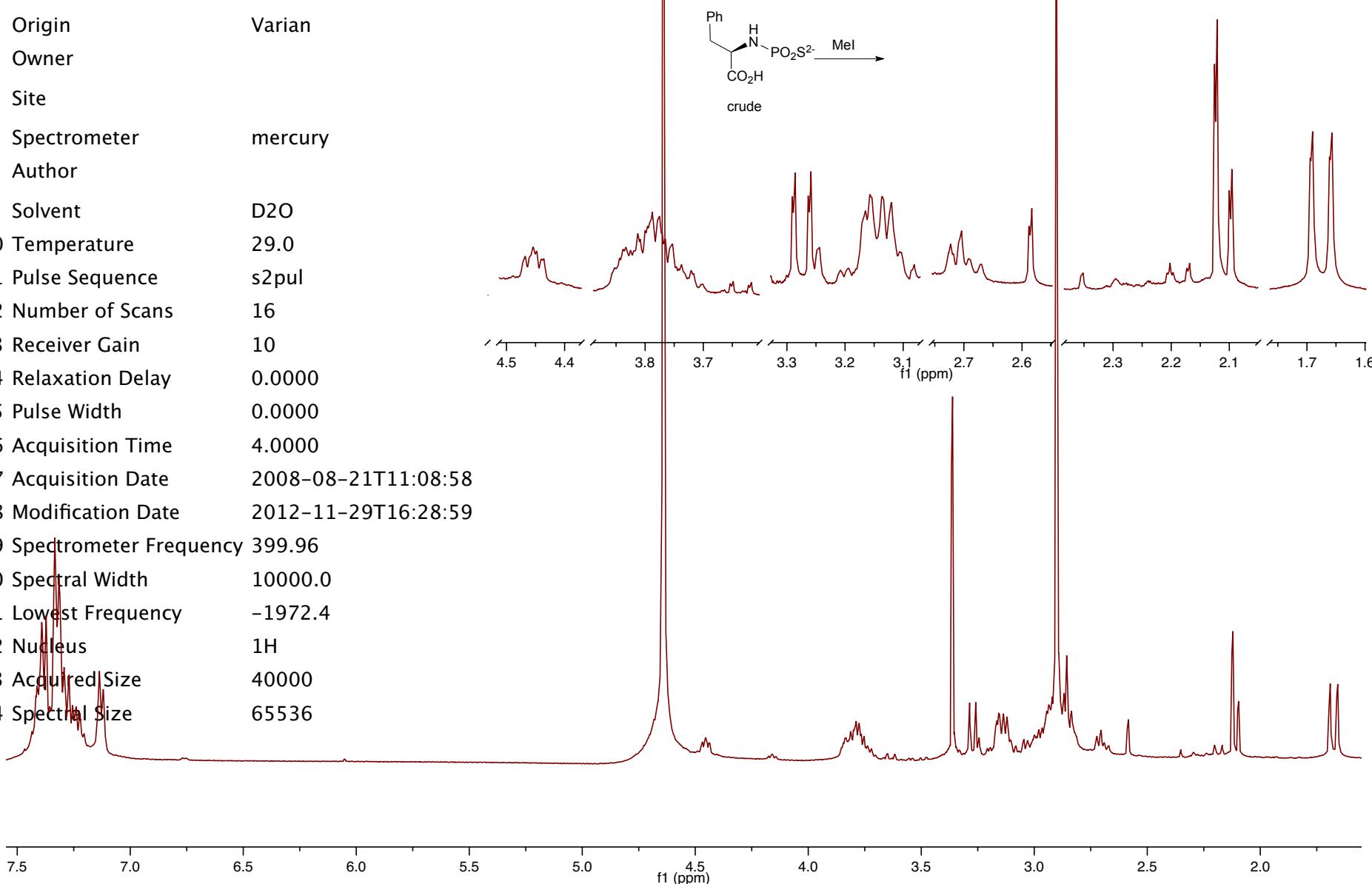
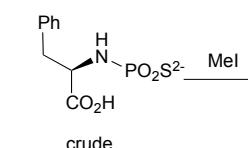
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4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	mercury
8 Author	
9 Solvent	D2O
10 Temperature	29.0
11 Pulse Sequence	s2pul
12 Number of Scans	128
13 Receiver Gain	34
14 Relaxation Delay	2.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.0000
17 Acquisition Date	2008-08-19T10:33:59
18 Modification Date	2012-11-29T16:28:59
19 Spectrometer Frequency	161.91
20 Spectral Width	50000.0
21 Lowest Frequency	-16535.8
22 Nucleus	31P
23 Acquired Size	50000
24 Spectral Size	65536



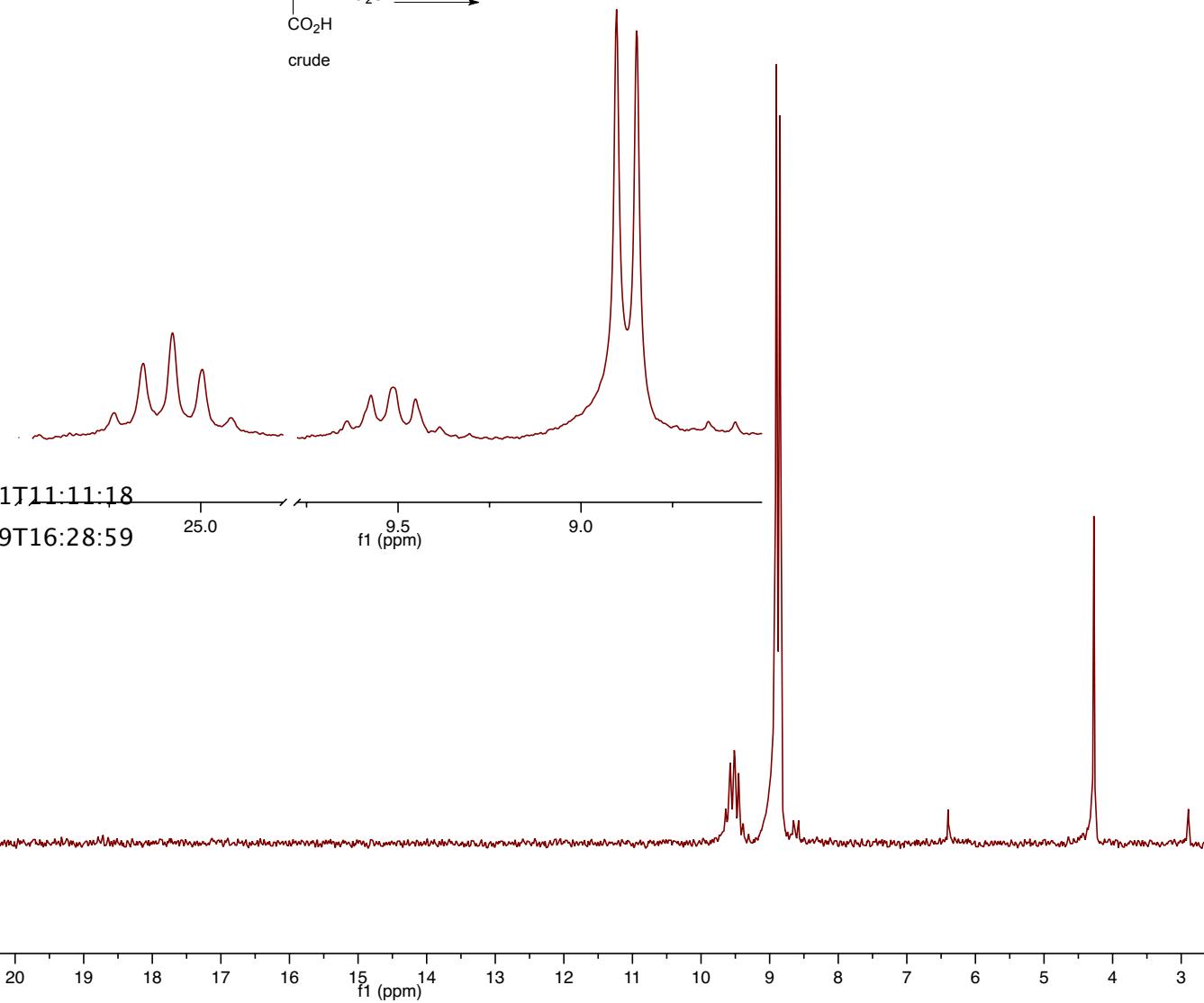
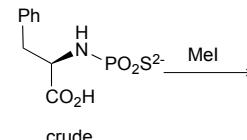
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5 Owner	
6 Site	
7 Spectrometer	mercury
8 Author	
9 Solvent	D2O
10 Temperature	29.0
11 Pulse Sequence	s2pul
12 Number of Scans	16
13 Receiver Gain	10
14 Relaxation Delay	0.0000
15 Pulse Width	0.0000
16 Acquisition Time	4.0000
17 Acquisition Date	2008-08-21T11:08:58
18 Modification Date	2012-11-29T16:28:59
19 Spectrometer Frequency	399.96
20 Spectral Width	10000.0
21 Lowest Frequency	-1972.4
22 Nucleus	1H
23 Acquired Size	40000
24 Spectral Size	65536

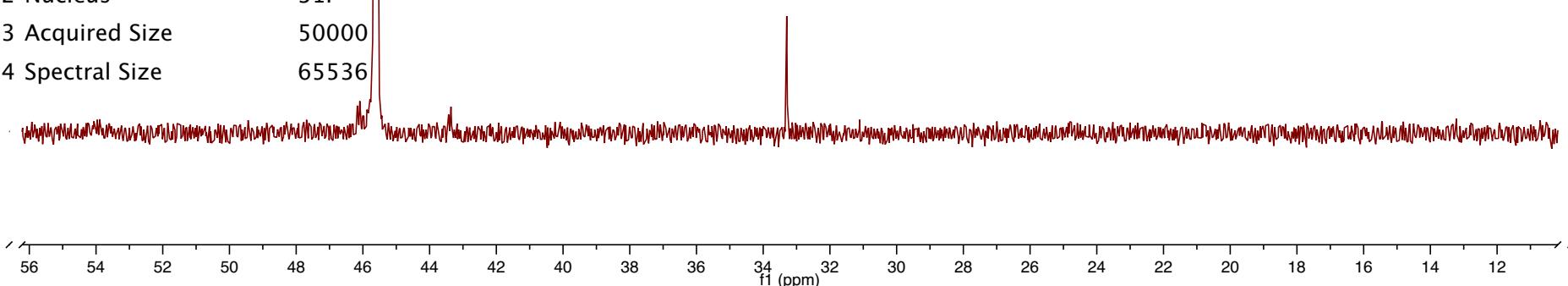
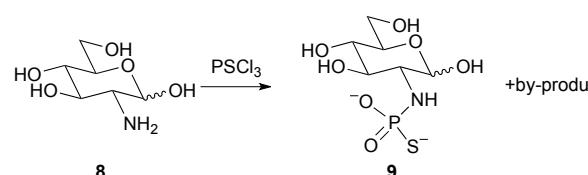
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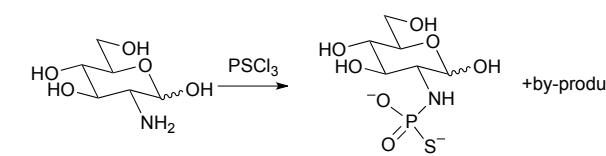
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4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	mercury
8 Author	
9 Solvent	D2O
10 Temperature	29.0
11 Pulse Sequence	s2pul
12 Number of Scans	64
13 Receiver Gain	34
14 Relaxation Delay	2.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.0000
17 Acquisition Date	2008-08-21T11:11:18
18 Modification Date	2012-11-29T16:28:59
19 Spectrometer Frequency	161.91
20 Spectral Width	50000.0
21 Lowest Frequency	-16535.8
22 Nucleus	^{31}P
23 Acquired Size	50000
24 Spectral Size	65536



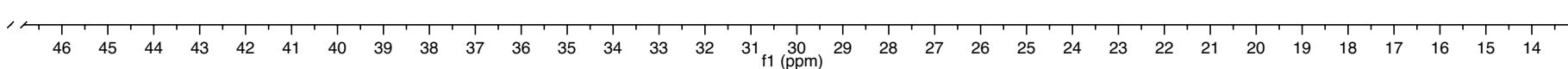
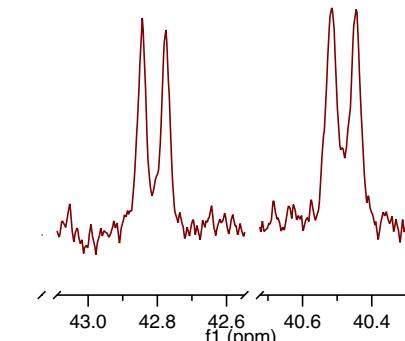
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3 Comment	MT376 thiophosph check
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	mercury
8 Author	
9 Solvent	D2O
10 Temperature	29.0
11 Pulse Sequence	s2pul
12 Number of Scans	80
13 Receiver Gain	34
14 Relaxation Delay	2.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.0000
17 Acquisition Date	2008-12-06T16:55:06
18 Modification Date	2012-08-28T16:51:08
19 Spectrometer Frequency	161.91
20 Spectral Width	50000.0
21 Lowest Frequency	-16535.8
22 Nucleus	³¹ P
23 Acquired Size	50000
24 Spectral Size	65536



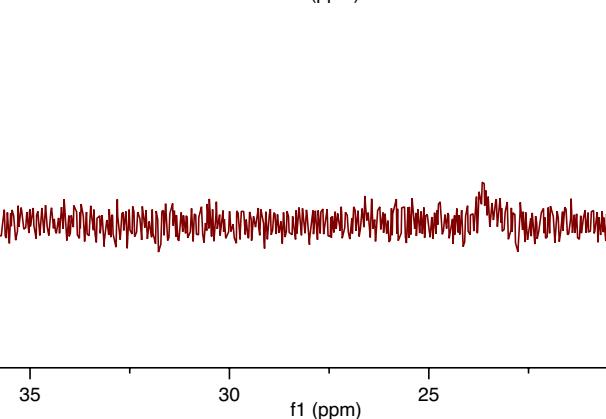
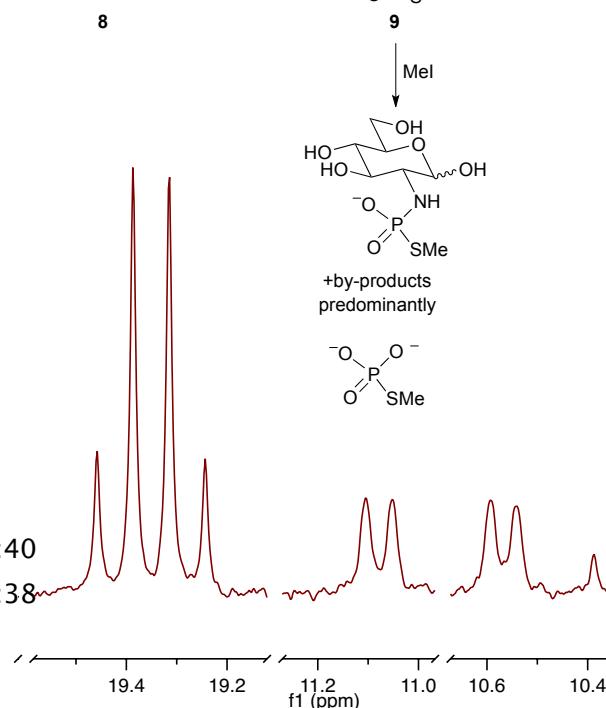
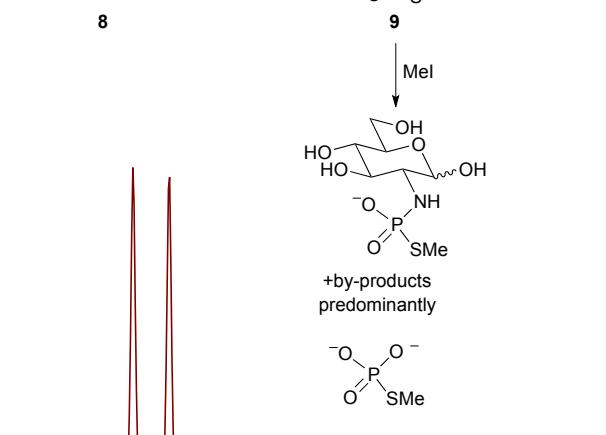
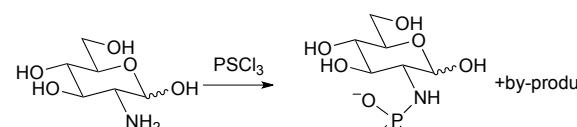
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3 Comment	MT376
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	mercury
8 Author	
9 Solvent	D2O
10 Temperature	29.0
11 Pulse Sequence	s2pul
12 Number of Scans	32
13 Receiver Gain	34
14 Relaxation Delay	2.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.0000
17 Acquisition Date	2008-12-06T18:15:21
18 Modification Date	2012-08-28T16:51:08
19 Spectrometer Frequency	161.91
20 Spectral Width	50000.0
21 Lowest Frequency	-16535.8
22 Nucleus	^{31}P
23 Acquired Size	50000
24 Spectral Size	65536



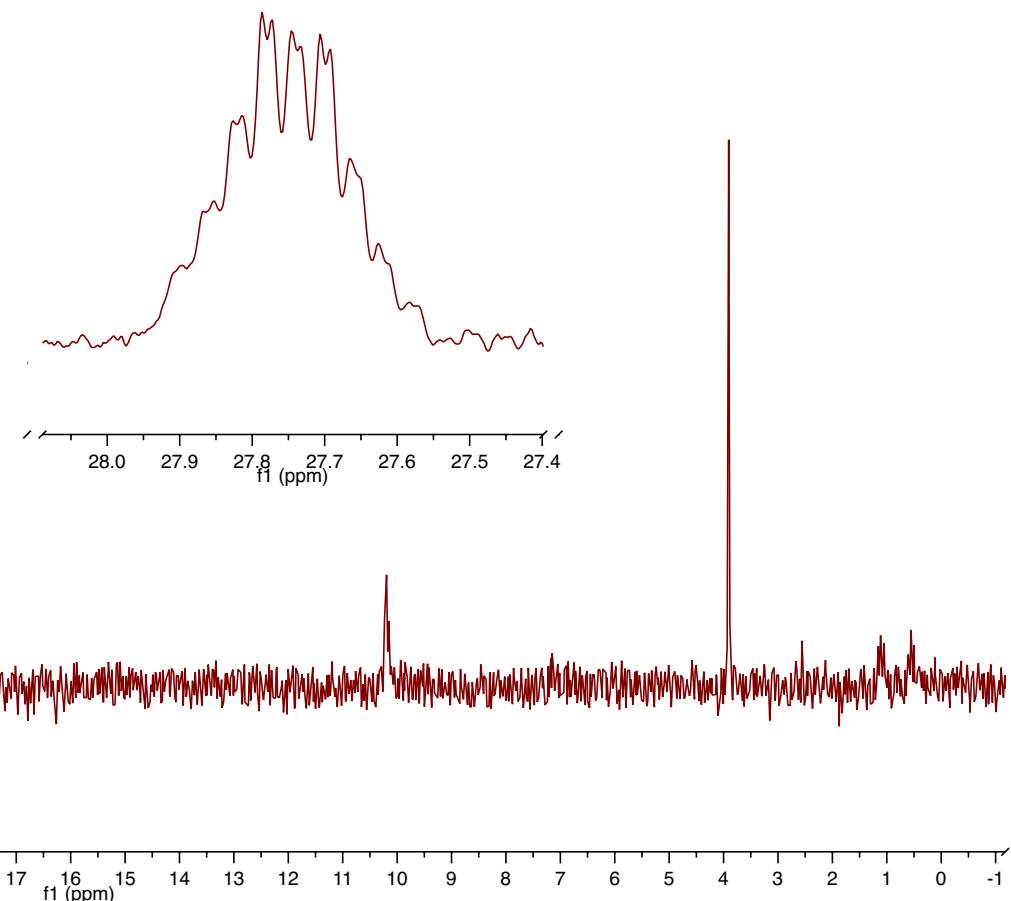
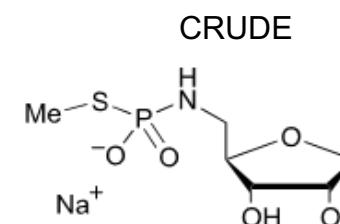
on standing for ~ 1 h



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4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	mercury
8 Author	
9 Solvent	D2O
10 Temperature	29.0
11 Pulse Sequence	s2pul
12 Number of Scans	64
13 Receiver Gain	34
14 Relaxation Delay	2.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.0000
17 Acquisition Date	2008-12-09T17:05:40
18 Modification Date	2012-08-28T17:34:38
19 Spectrometer Frequency	161.91
20 Spectral Width	50000.0
21 Lowest Frequency	-16535.8
22 Nucleus	³¹ P
23 Acquired Size	50000
24 Spectral Size	65536

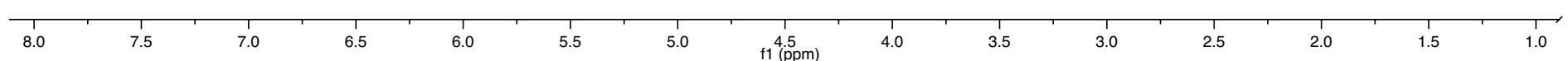
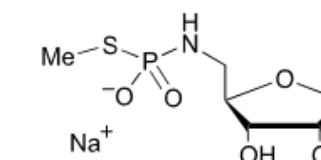


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4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	mercury
8 Author	
9 Solvent	D2O
10 Temperature	29.0
11 Pulse Sequence	s2pul
12 Number of Scans	96
13 Receiver Gain	36
14 Relaxation Delay	2.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.0000
17 Acquisition Date	2009-02-02T19:43:08
18 Modification Date	2012-11-06T16:03:21
19 Spectrometer Frequency	161.91
20 Spectral Width	50000.0
21 Lowest Frequency	-16535.8
22 Nucleus	³¹ P
23 ACF width (ppm)	50000
24 Spectral Size	65536

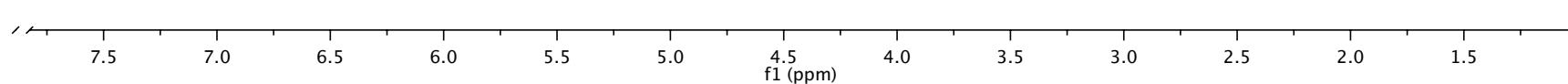


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6 Site	
7 Spectrometer	mercury
8 Author	
9 Solvent	D2O
10 Temperature	29.0
11 Pulse Sequence	s2pul
12 Number of Scans	16
13 Receiver Gain	20
14 Relaxation Delay	0.0000
15 Pulse Width	0.0000
16 Acquisition Time	4.0000
17 Acquisition Date	2009-02-02T19:49:39
18 Modification Date	2012-11-06T16:03:21
19 Spectrometer Frequency	399.96
20 Spectral Width	10000.0
21 Lowest Frequency	-1972.4
22 Nucleus	1H
23 Acquired Size	40000
24 Spectral Size	65536

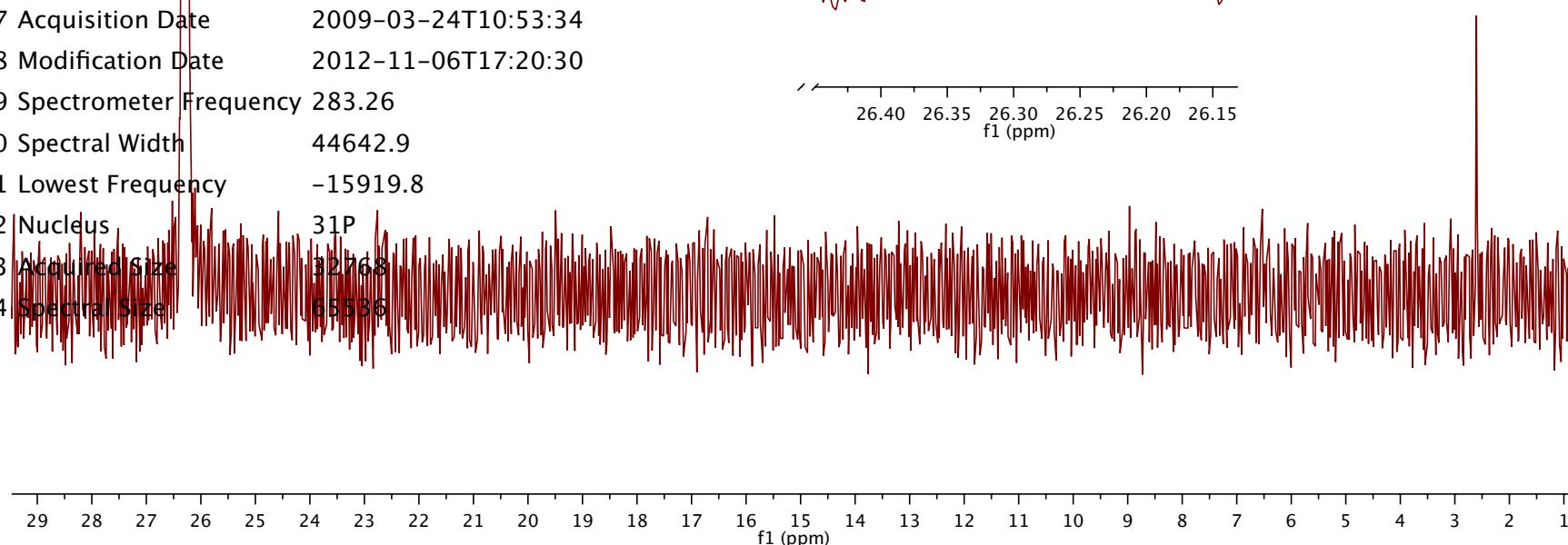
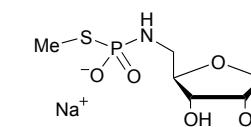
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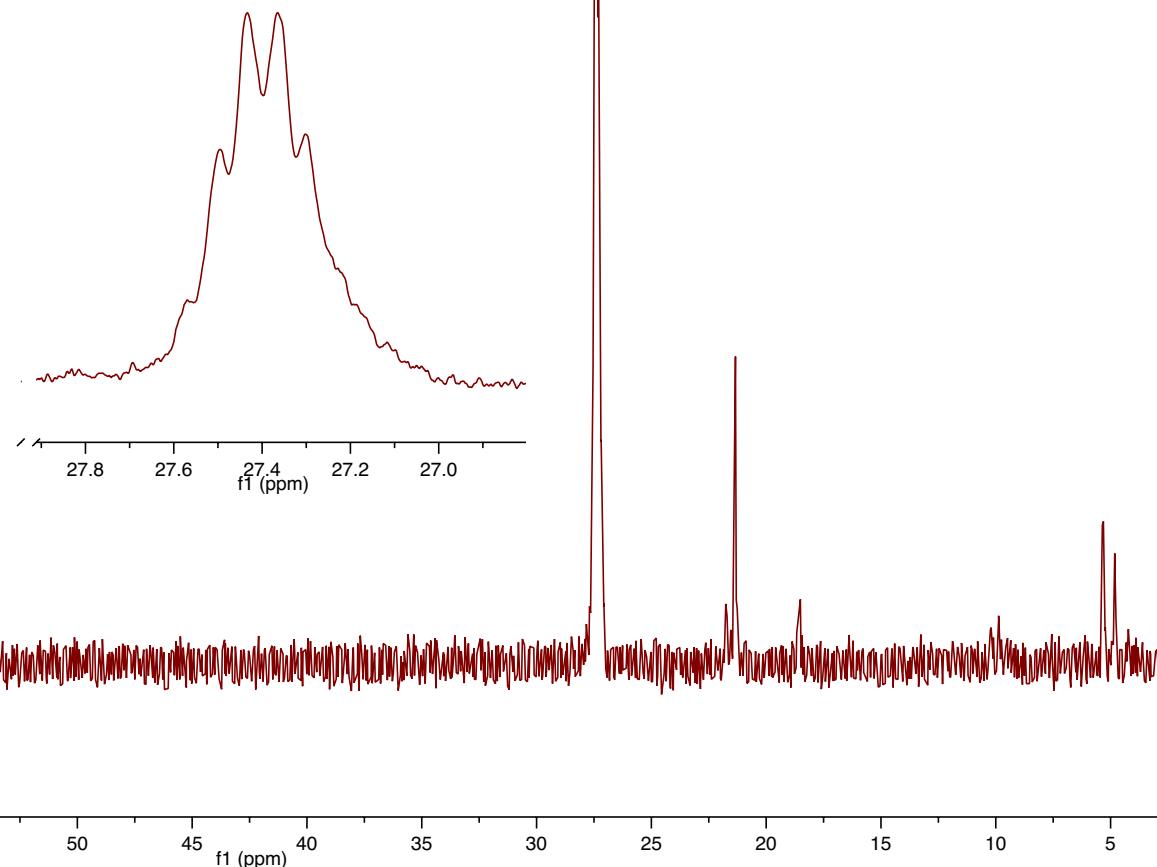
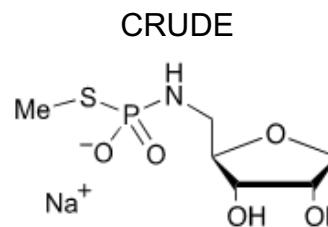
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3 Comment	MT 465
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	d2o
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	4
13 Receiver Gain	44
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	2.9098
17 Acquisition Date	2009-03-23T16:02:35
18 Modification Date	2012-11-06T17:20:28
19 Spectrometer Frequency	699.74
20 Spectral Width	11261.3
21 Lowest Frequency	-1432.2
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536



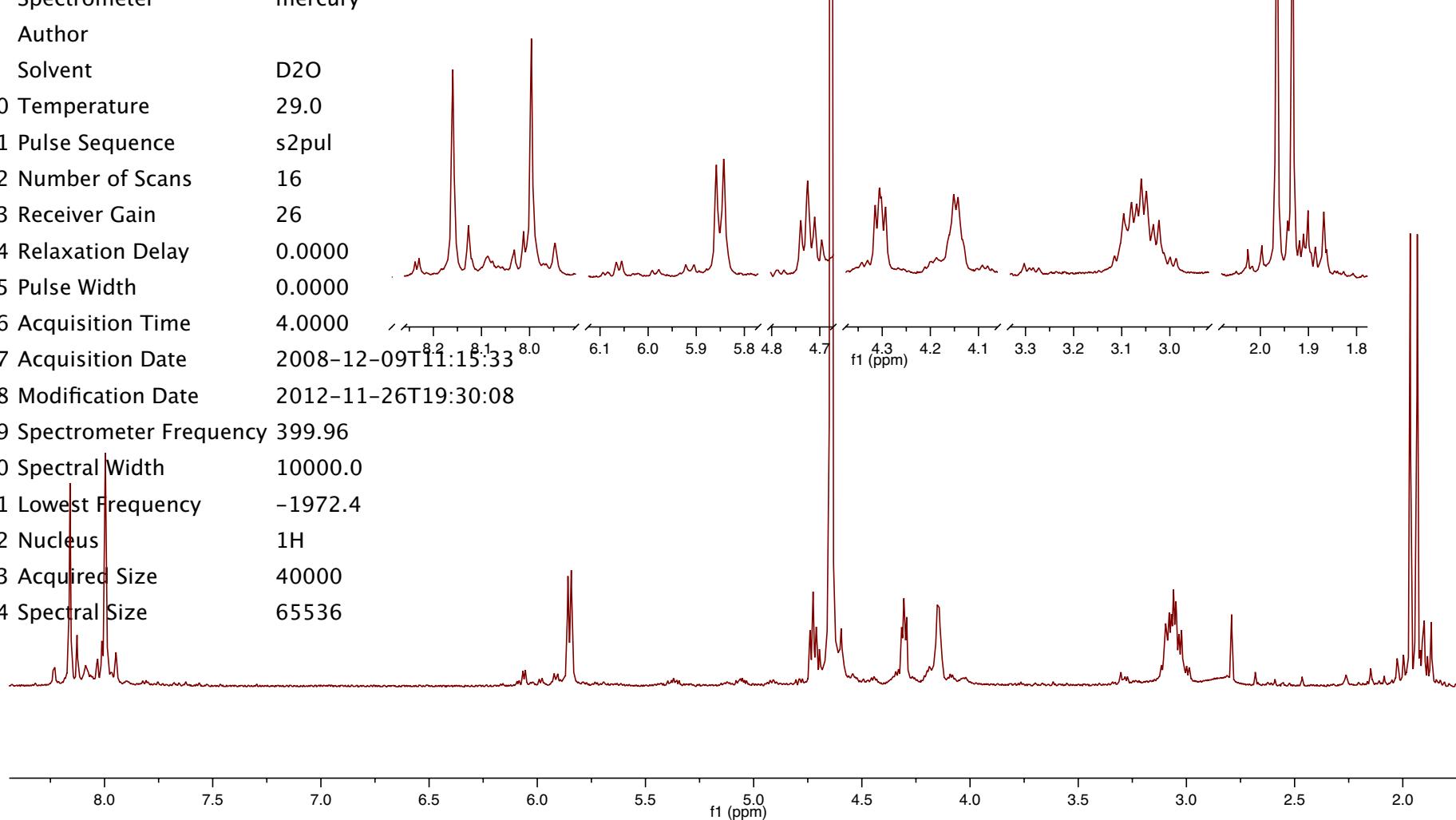
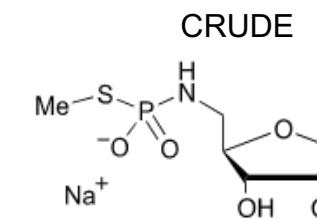
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3 Comment	MT 465
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	d2o
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	256
13 Receiver Gain	50
14 Relaxation Delay	3.0000
15 Pulse Width	0.0000
16 Acquisition Time	0.7340
17 Acquisition Date	2009-03-24T10:53:34
18 Modification Date	2012-11-06T17:20:30
19 Spectrometer Frequency	283.26
20 Spectral Width	44642.9
21 Lowest Frequency	-15919.8
22 Nucleus	^{31}P
23 Acquired Size	32768
24 Spectral Size	65536



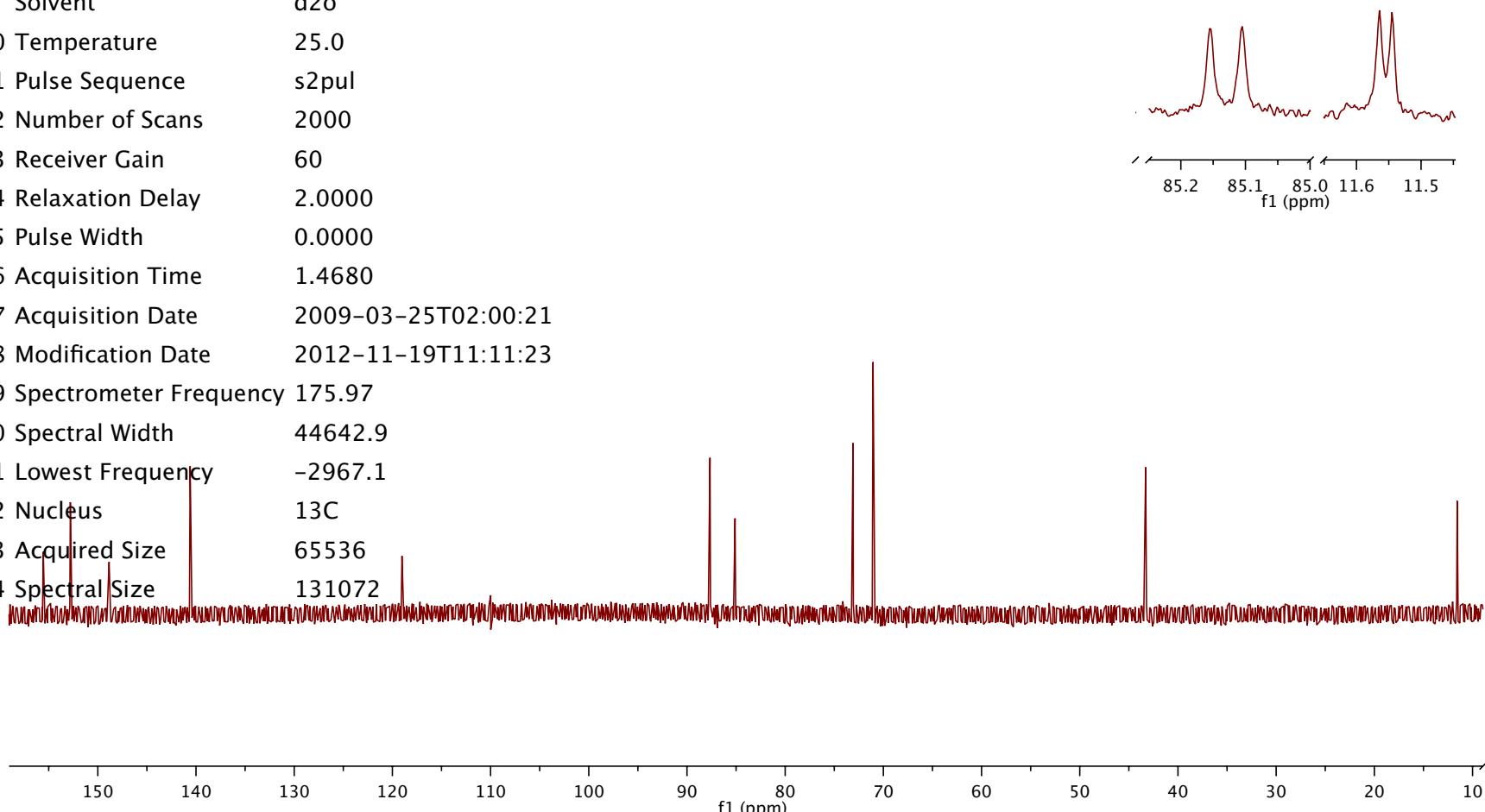
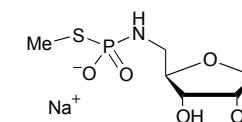
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5 Owner	
6 Site	
7 Spectrometer	mercury
8 Author	
9 Solvent	D2O
10 Temperature	29.0
11 Pulse Sequence	s2pul
12 Number of Scans	128
13 Receiver Gain	34
14 Relaxation Delay	2.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.0000
17 Acquisition Date	2008-12-09T11:22:59
18 Modification Date	2012-11-26T19:30:08
19 Spectrometer Frequency	161.91
20 Spectral Width	50000.0
21 Lowest Frequency	-16535.8
22 Nucleus	^{31}P
23 Acquired Size	50000
24 Spectral Size	65536



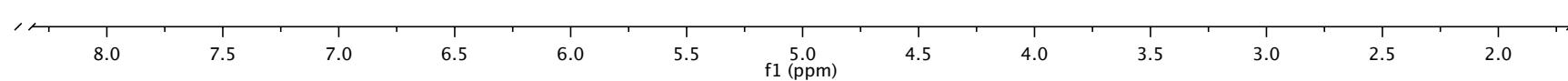
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5 Owner	
6 Site	
7 Spectrometer	mercury
8 Author	
9 Solvent	D2O
10 Temperature	29.0
11 Pulse Sequence	s2pul
12 Number of Scans	16
13 Receiver Gain	26
14 Relaxation Delay	0.0000
15 Pulse Width	0.0000
16 Acquisition Time	4.0000
17 Acquisition Date	2008-12-09T11:15:33
18 Modification Date	2012-11-26T19:30:08
19 Spectrometer Frequency	399.96
20 Spectral Width	10000.0
21 Lowest Frequency	-1972.4
22 Nucleus	1H
23 Acquired Size	40000
24 Spectral Size	65536



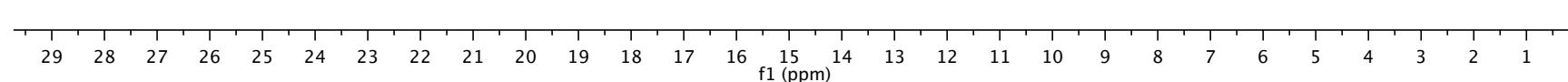
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5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	d2o
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	2000
13 Receiver Gain	60
14 Relaxation Delay	2.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.4680
17 Acquisition Date	2009-03-25T02:00:21
18 Modification Date	2012-11-19T11:11:23
19 Spectrometer Frequency	175.97
20 Spectral Width	44642.9
21 Lowest Frequency	-2967.1
22 Nucleus	¹³ C
23 Acquired Size	65536
24 Spectral Size	131072



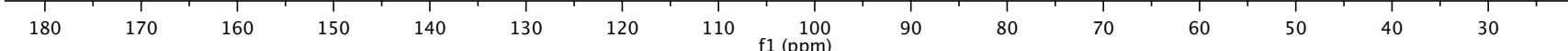
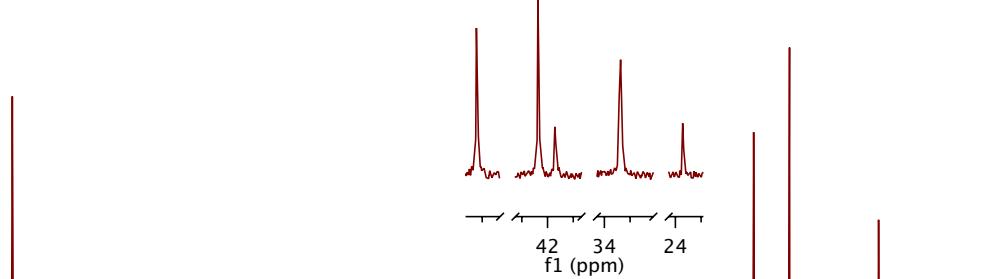
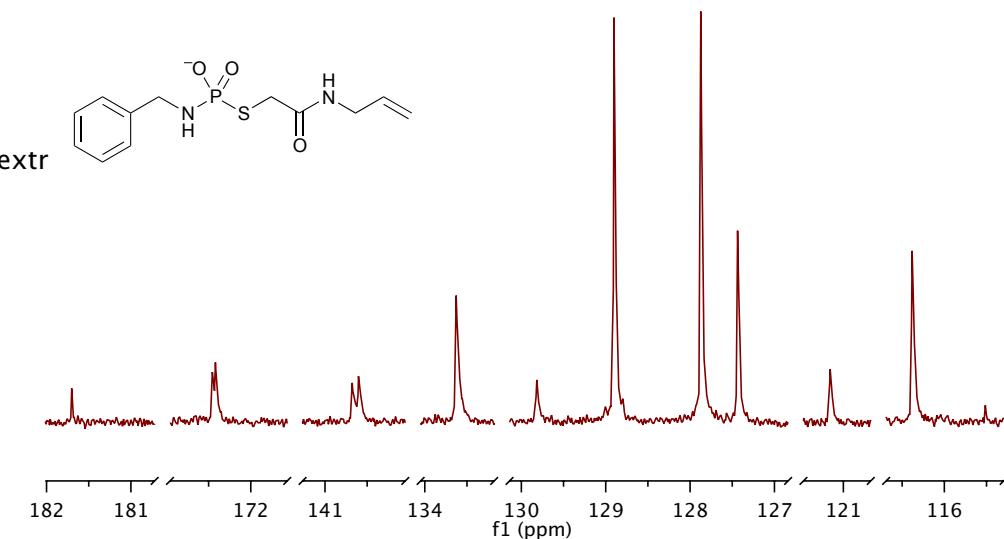
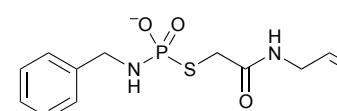
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4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	d2o
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	4
13 Receiver Gain	42
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	2.9098
17 Acquisition Date	2009-03-23T15:57:55
18 Modification Date	2012-11-19T11:11:22
19 Spectrometer Frequency	699.74
20 Spectral Width	11261.3
21 Lowest Frequency	-1432.2
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536



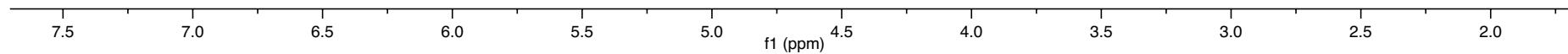
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3 Comment	MT 378
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	d2o
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	256
13 Receiver Gain	50
14 Relaxation Delay	3.0000
15 Pulse Width	0.0000
16 Acquisition Time	0.7340
17 Acquisition Date	2009-03-24T10:33:18
18 Modification Date	2012-11-19T11:11:22
19 Spectrometer Frequency	283.26
20 Spectral Width	44642.9
21 Lowest Frequency	-15919.8
22 Nucleus	^{31}P
23 Acquired Size	32768
24 Spectral Size	65536



Parameter	Value
1 Data File Name	C:/ Documents and Settings/ Owner/ My Documents/ Dropbox/ Milena OBC/ NMR files (unprocessed)/ MT496/ 20120631/ 11/ fid
2 Title	20120631
3 Comment	RGL drwh Owner milena trmcic MT496 freeze dried+CDCl ₃ extr
4 Origin	Bruker BioSpin GmbH
5 Owner	otto
6 Site	av400
7 Spectrometer	
8 Author	
9 Solvent	D ₂ O
10 Temperature	297.2
11 Pulse Sequence	zgpg30
12 Number of Scans	1024
13 Receiver Gain	20642
14 Relaxation Delay	2.0000
15 Pulse Width	8.0000
16 Acquisition Time	1.3665
17 Acquisition Date	2009-02-20T22:33:00
18 Modification Date	2012-11-20T16:03:59
19 Spectrometer Frequency	100.62
20 Spectral Width	23980.8
21 Lowest Frequency	-1929.6
22 Nucleus	¹³ C
23 Acquired Size	32709
24 Specified Size	15000



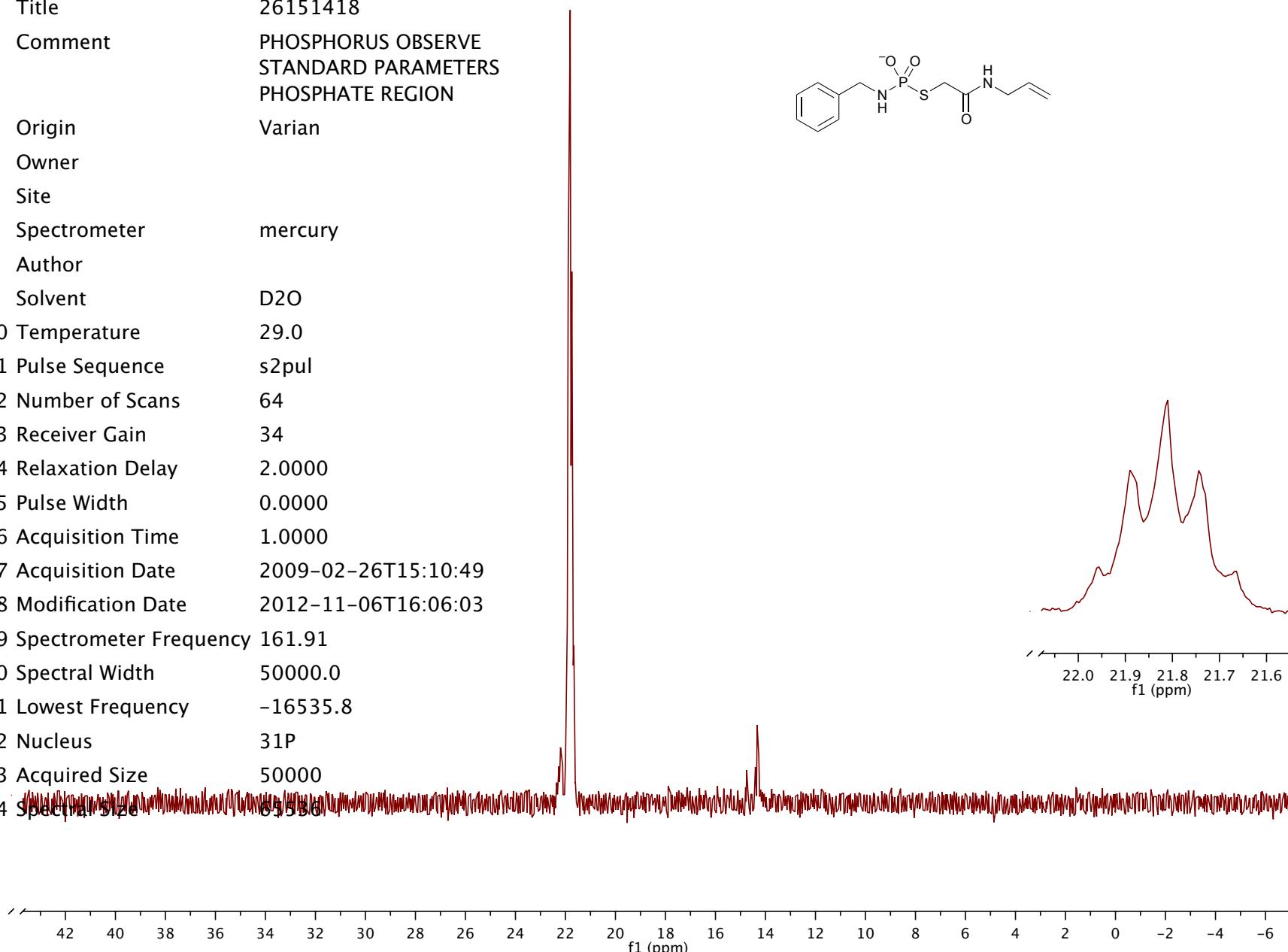
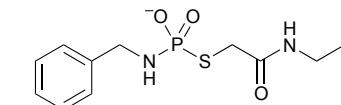
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4 Origin	Bruker BioSpin GmbH
5 Owner	otto
6 Site	
7 Spectrometer	av400
8 Author	
9 Solvent	D2O
10 Temperature	295.2
11 Pulse Sequence	zg30
12 Number of Scans	16
13 Receiver Gain	72
14 Relaxation Delay	1.0000
15 Pulse Width	9.5000
16 Acquisition Time	3.9584
17 Acquisition Date	2009-02-26T14:29:00
18 Modification Date	2012-11-06T17:43:34
19 Spectrometer Frequency	400.13
20 Spectral Width	8278.1
21 Lowest Frequency	-1668.1
22 Nucleus	1H
23 Acquired Size	32696
24 Spectral Size	65536



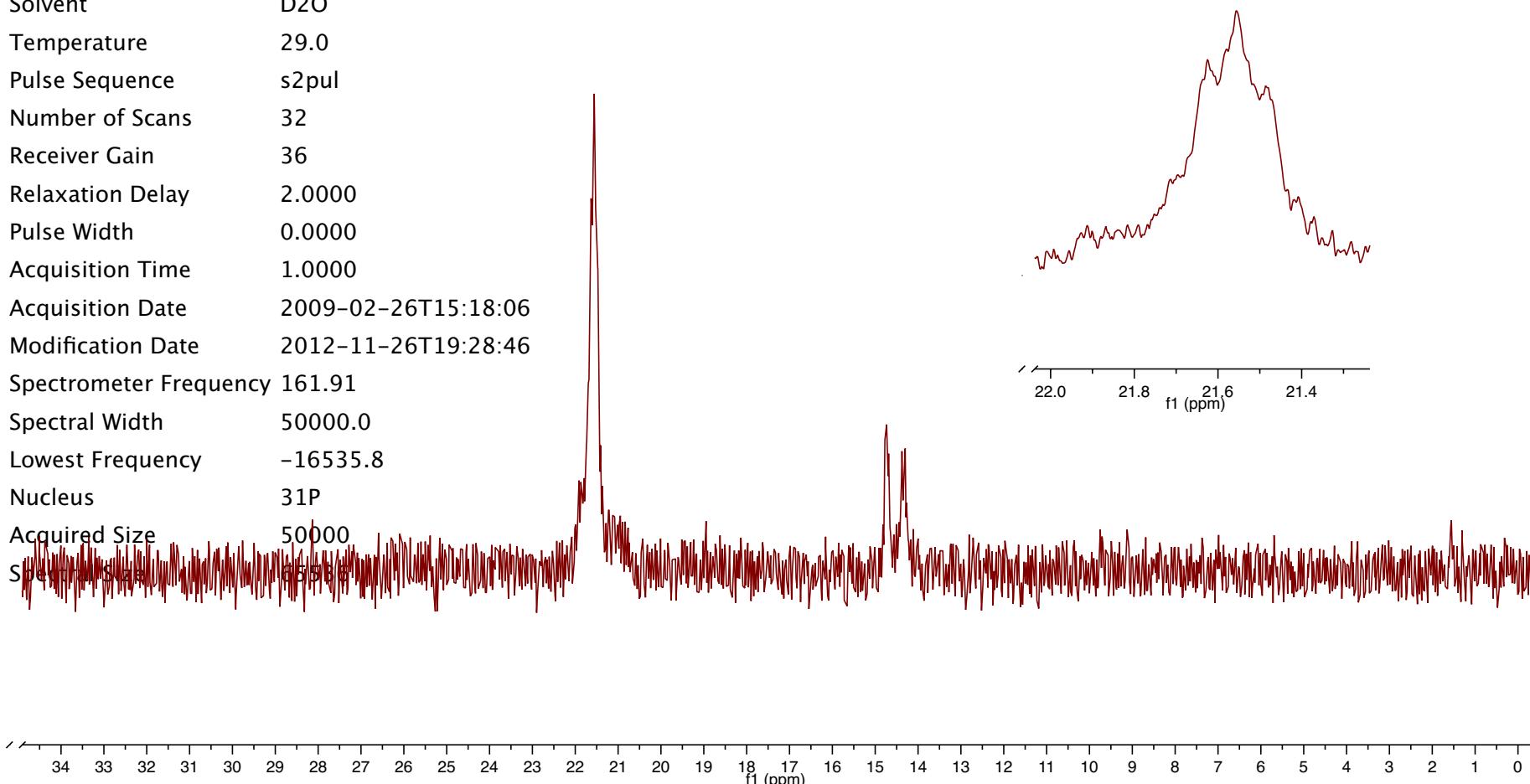
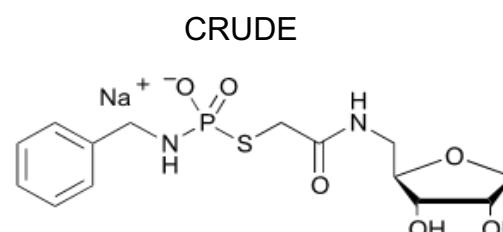
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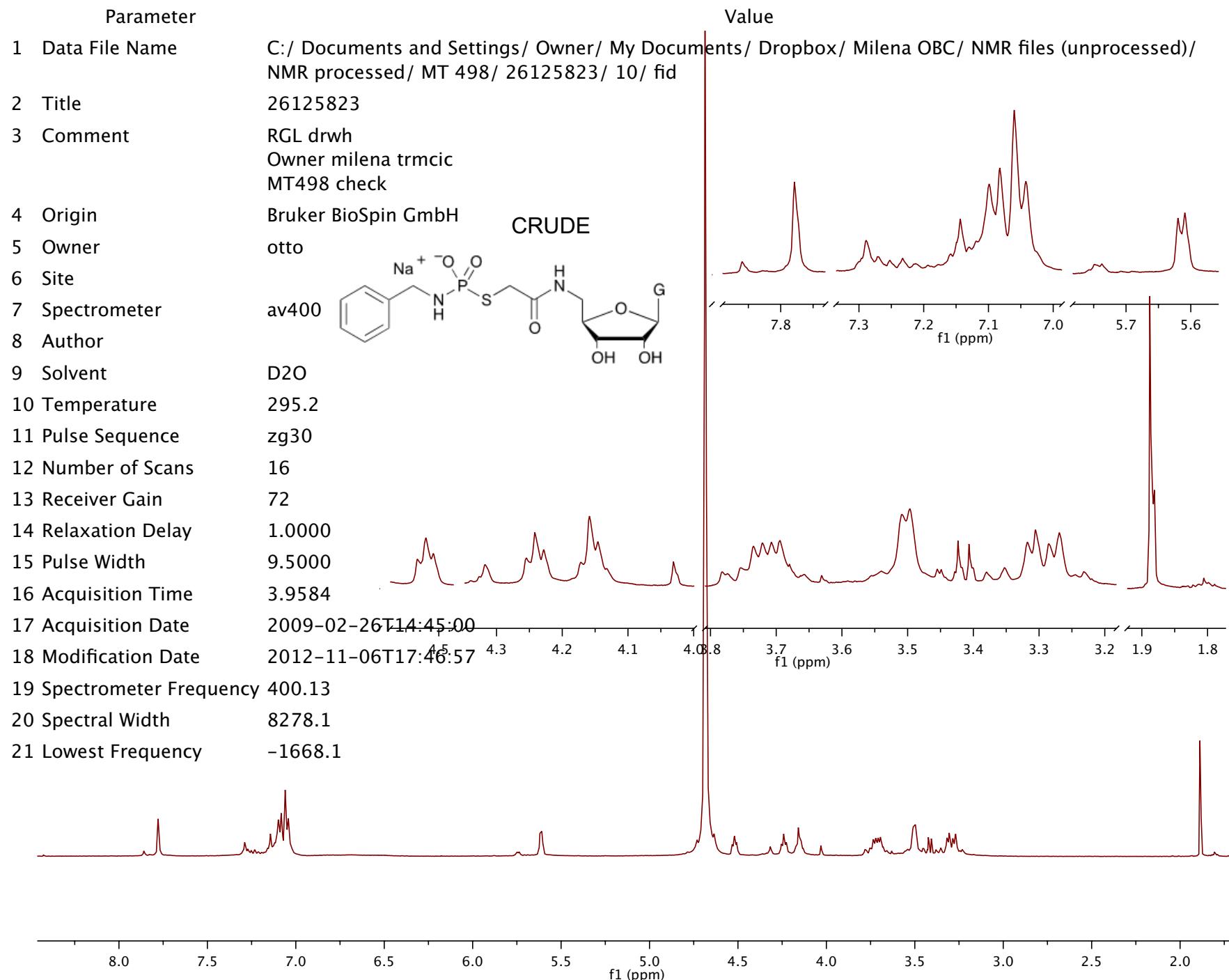
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4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	mercury
8 Author	
9 Solvent	D2O
10 Temperature	29.0
11 Pulse Sequence	s2pul
12 Number of Scans	64
13 Receiver Gain	34
14 Relaxation Delay	2.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.0000
17 Acquisition Date	2009-02-26T15:10:49
18 Modification Date	2012-11-06T16:06:03
19 Spectrometer Frequency	161.91
20 Spectral Width	50000.0
21 Lowest Frequency	-16535.8
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23 Acquired Size	50000
24 Spectral Size	65536

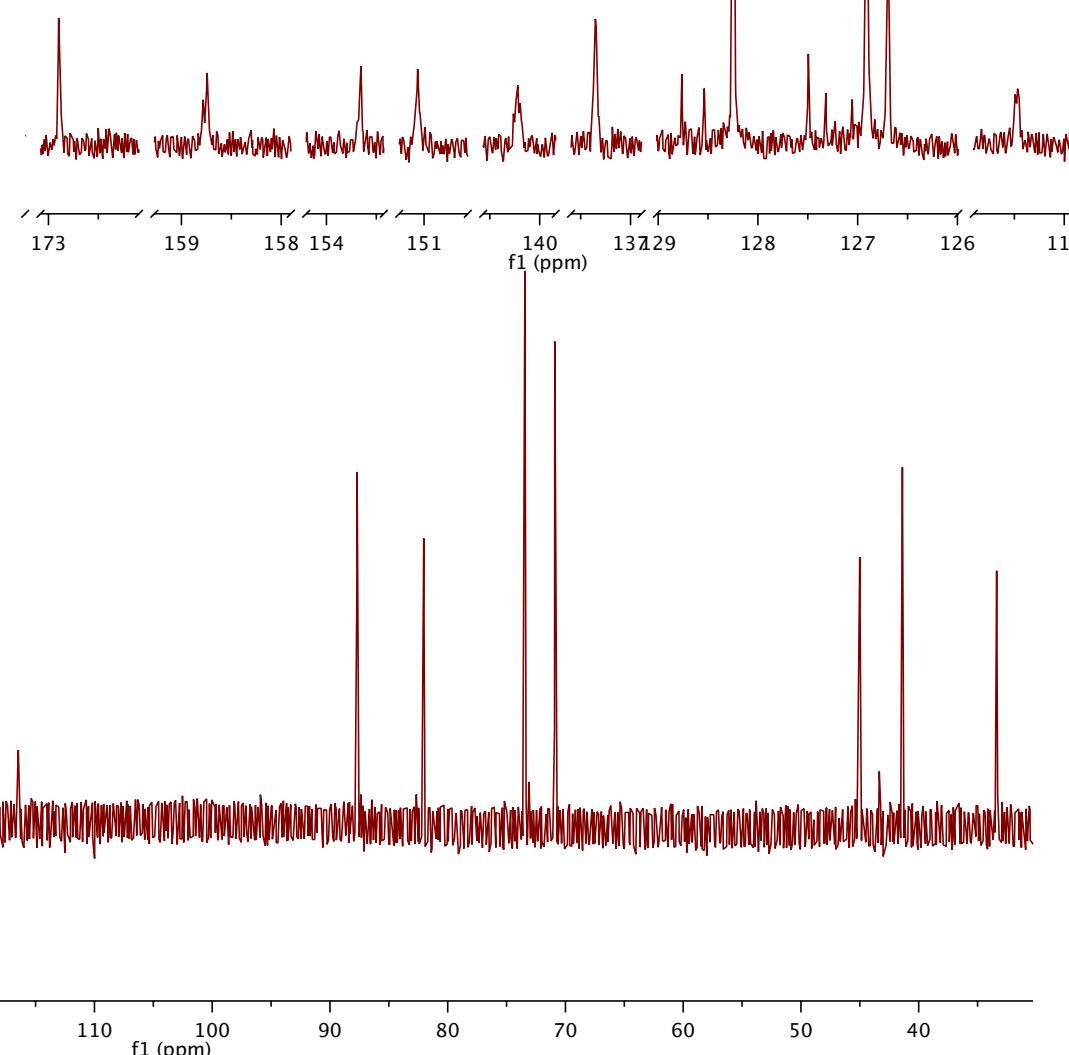
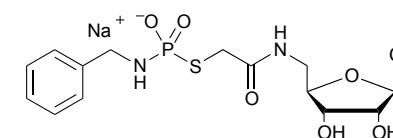


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8 Author	
9 Solvent	D2O
10 Temperature	29.0
11 Pulse Sequence	s2pul
12 Number of Scans	32
13 Receiver Gain	36
14 Relaxation Delay	2.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.0000
17 Acquisition Date	2009-02-26T15:18:06
18 Modification Date	2012-11-26T19:28:46
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22 Nucleus	31P
23 Acquired Size	50000
24 Spec. Size	50000

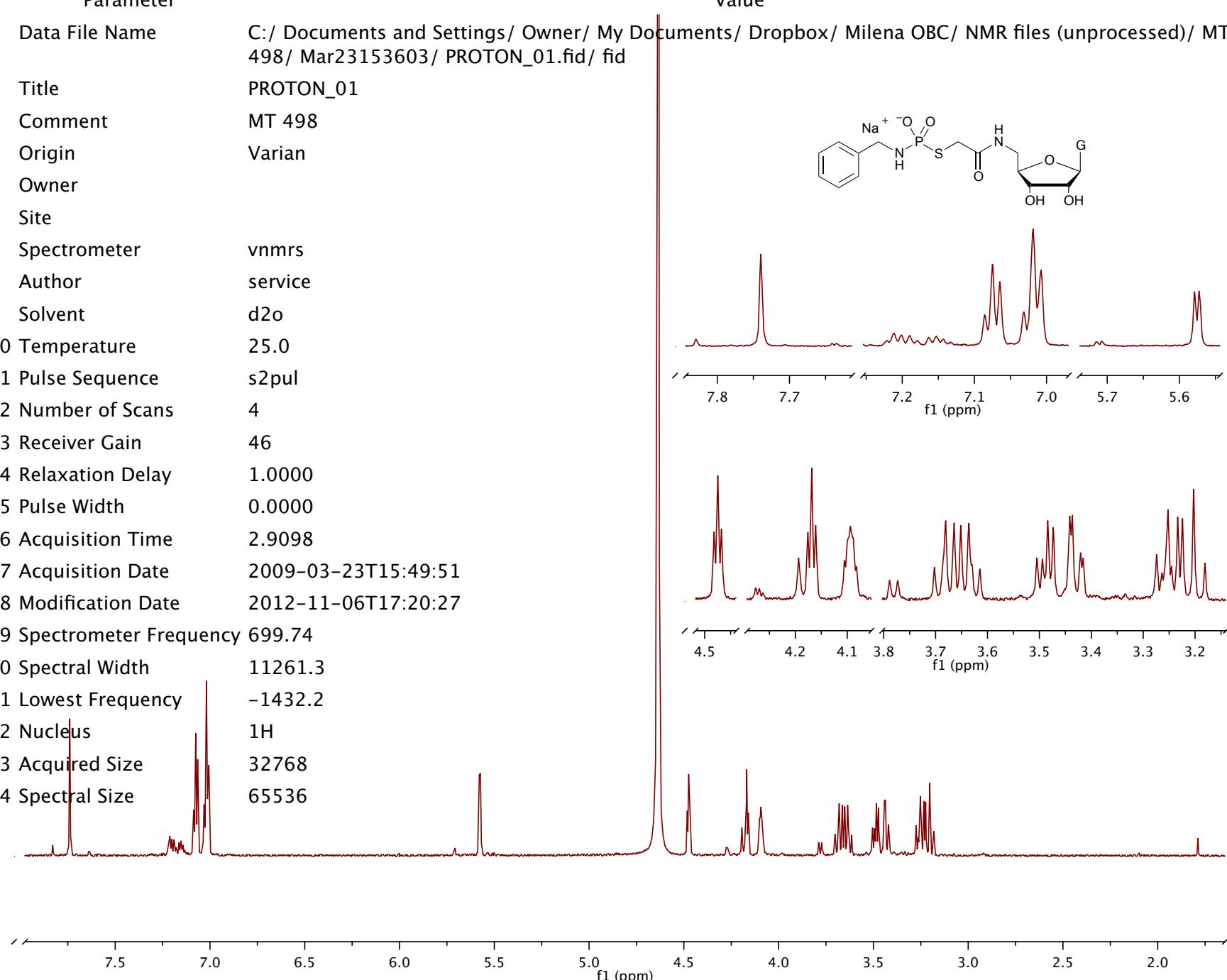




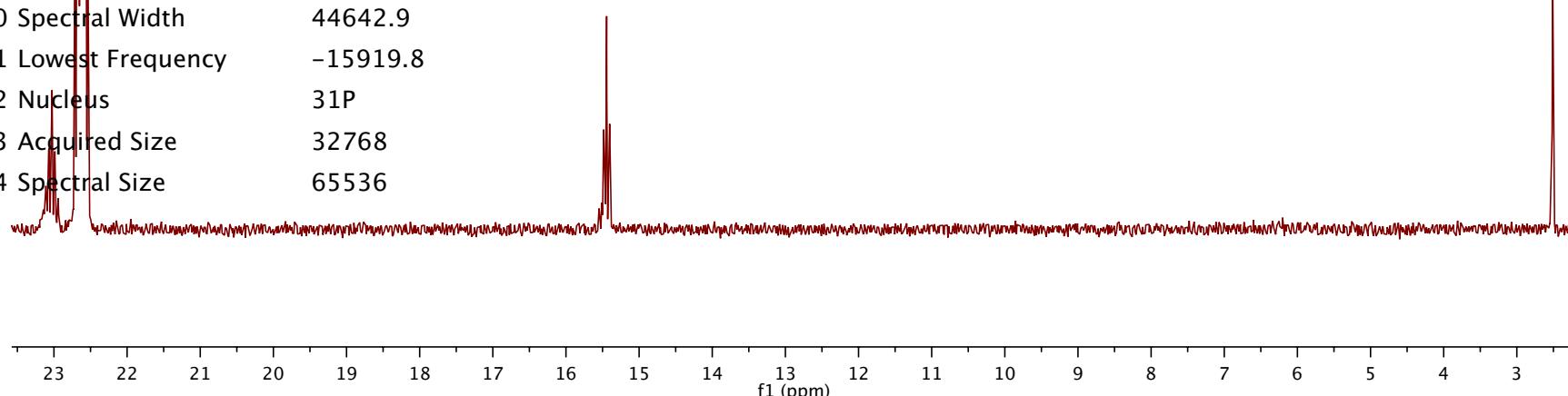
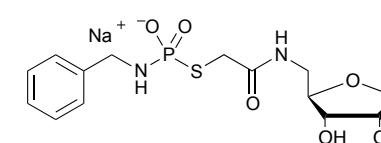
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3 Comment	MT 498
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	d2o
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	2000
13 Receiver Gain	60
14 Relaxation Delay	2.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.4680
17 Acquisition Date	2009-03-24T22:02:03
18 Modification Date	2012-11-06T17:20:32
19 Spectrometer Frequency	175.97
20 Spectral Width	44642.9
21 Lowest Frequency	-2967.1
22 Nucleus	¹³ C
23 Acquired Size	65536
24 Spectral Size	131072

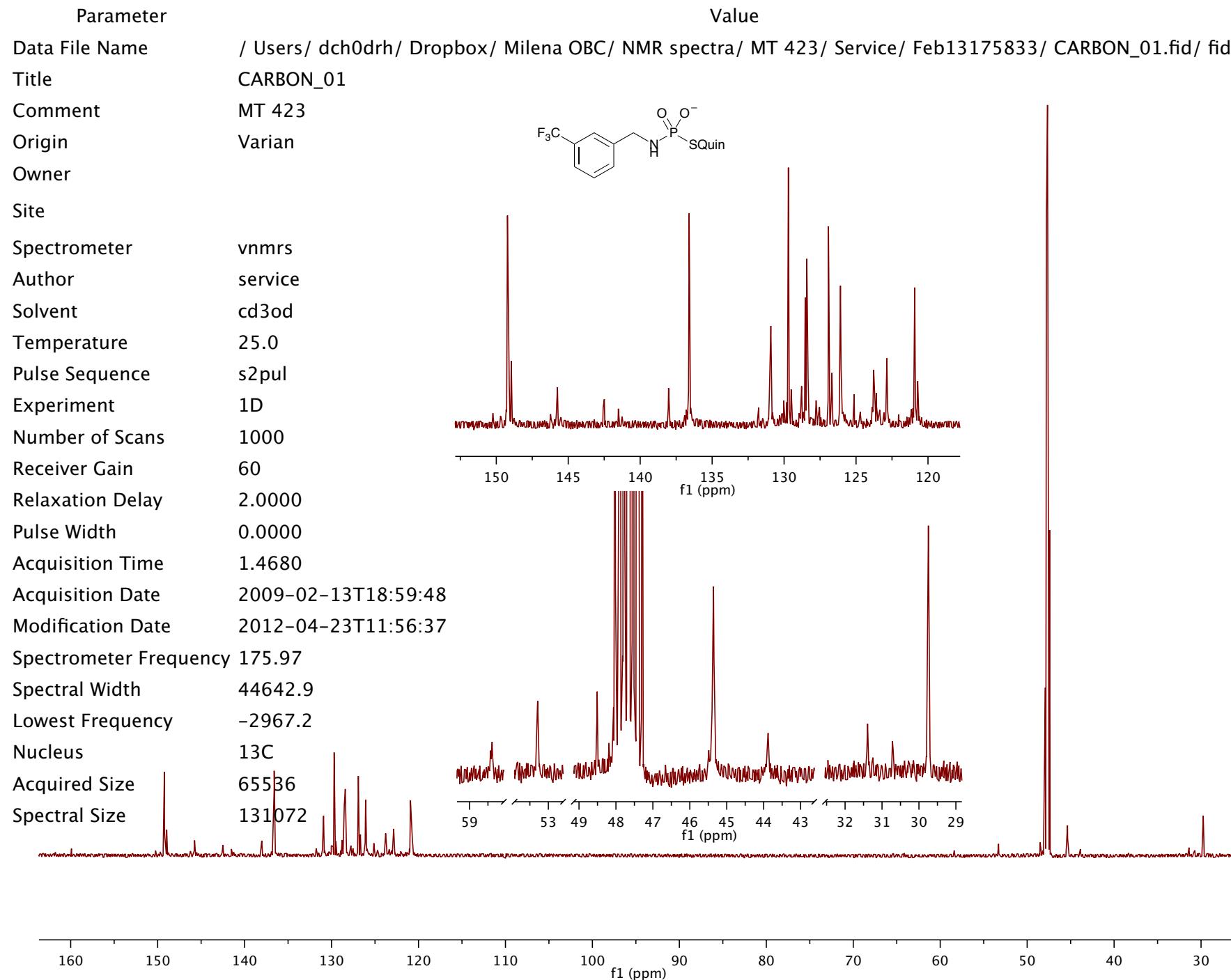


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5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	d2o
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	4
13 Receiver Gain	46
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	2.9098
17 Acquisition Date	2009-03-23T15:49:51
18 Modification Date	2012-11-06T17:20:27
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20 Spectral Width	11261.3
21 Lowest Frequency	-1432.2
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536

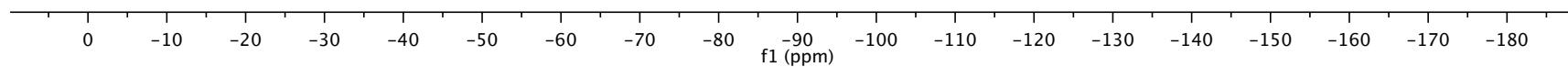
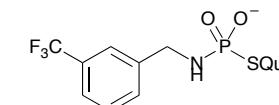


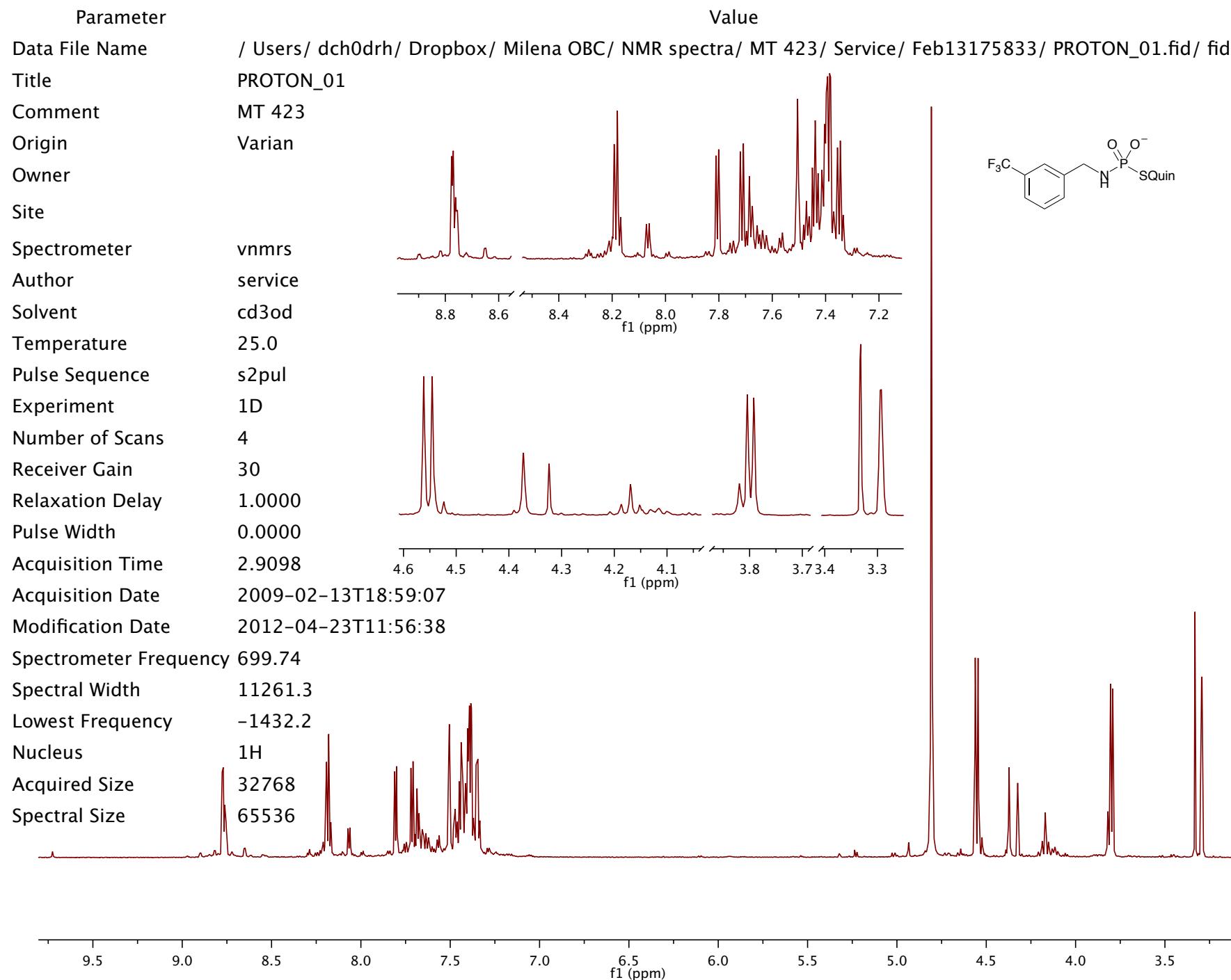
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3 Comment	MT 498
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5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	d2o
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	256
13 Receiver Gain	50
14 Relaxation Delay	3.0000
15 Pulse Width	0.0000
16 Acquisition Time	0.7340
17 Acquisition Date	2009-03-24T09:53:17
18 Modification Date	2012-11-06T17:20:30
19 Spectrometer Frequency	283.26
20 Spectral Width	44642.9
21 Lowest Frequency	-15919.8
22 Nucleus	^{31}P
23 Acquired Size	32768
24 Spectral Size	65536

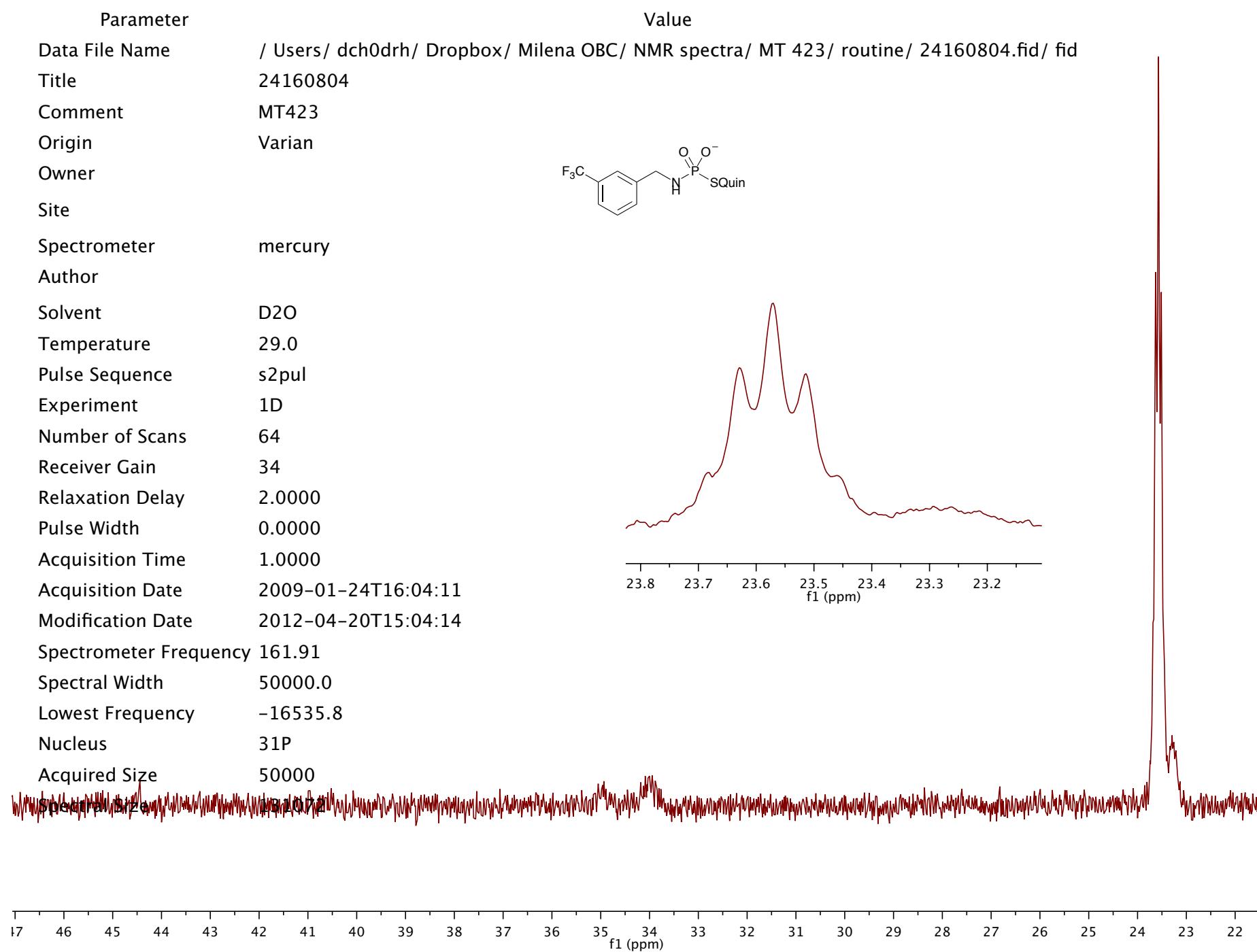




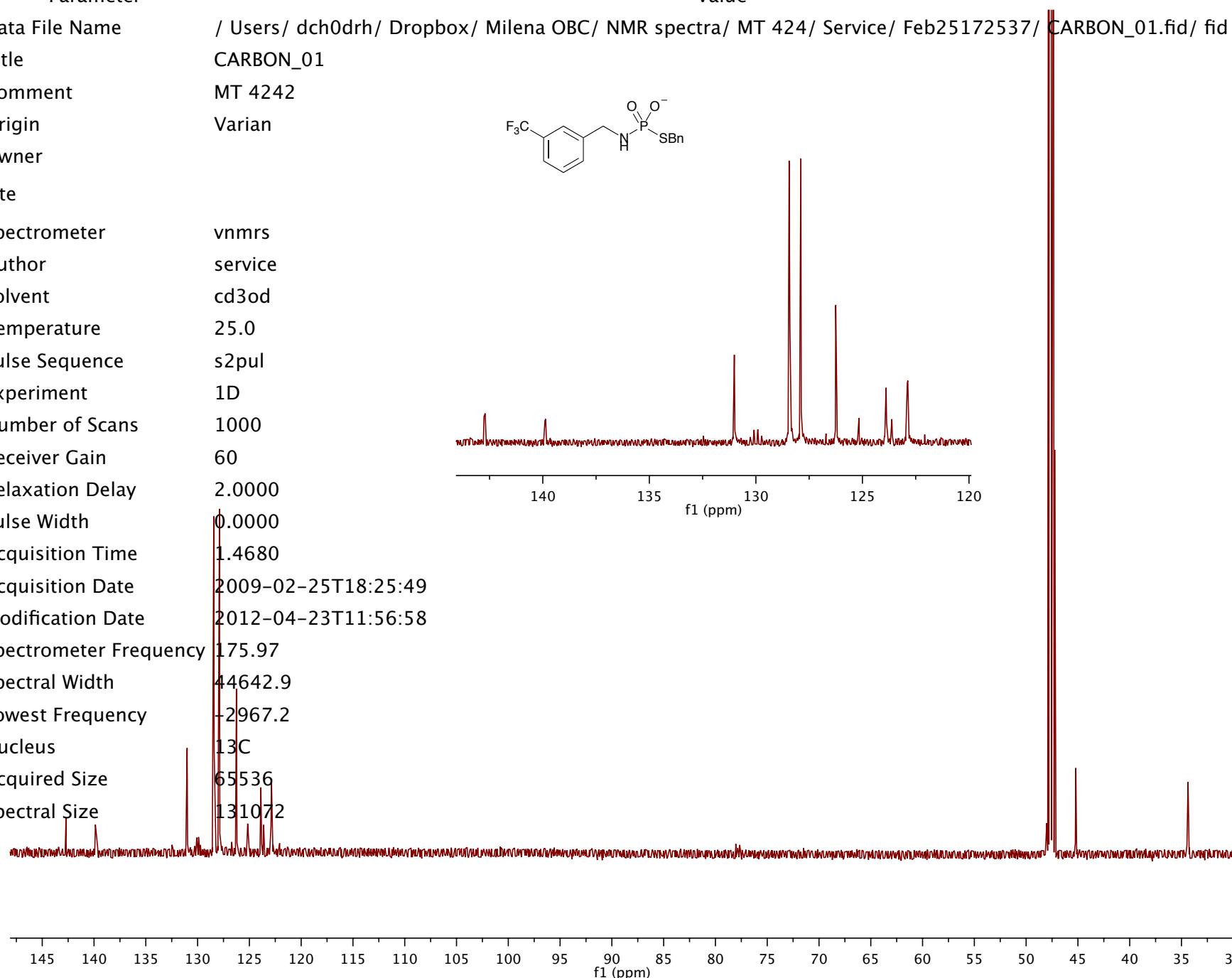
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2 Title	11124230
3 Comment	RGL DRWH Owner Milena Trmcic MT 423
4 Origin	Bruker BioSpin GmbH
5 Owner	Administrator
6 Site	
7 Spectrometer	av400
8 Author	
9 Solvent	MeOD
10 Temperature	293.1
11 Pulse Sequence	zgflqn
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	1024
15 Relaxation Delay	2.0000
16 Pulse Width	11.8000
17 Acquisition Time	0.8717
18 Acquisition Date	2009-05-11T12:55:00
19 Modification Date	2012-04-20T15:17:52
20 Spectrometer Frequency	376.39
21 Spectral Width	75188.0
22 Lowest Frequency	-71472.1
23 Nucleus	¹⁹ F
24 Acquired Size	65536
25 Spectral Size	131072



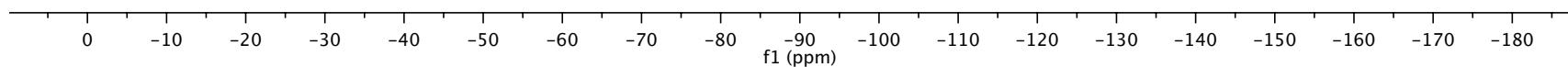
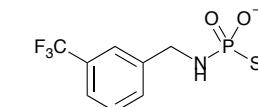


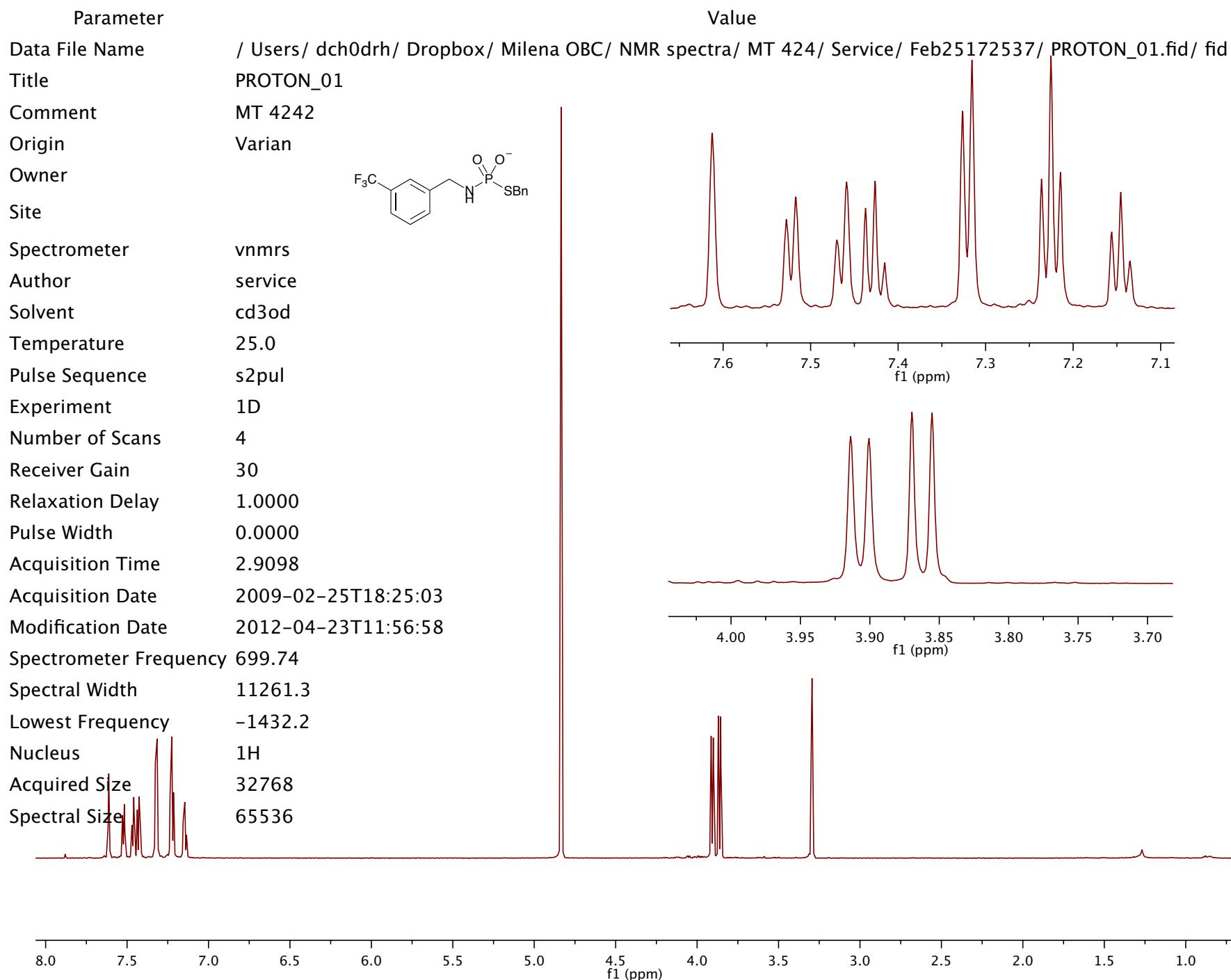


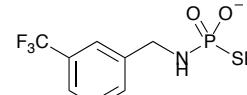
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Origin	Varian
Owner	
Site	
Spectrometer	vnmrs
Author	service
Solvent	cd3od
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	1000
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.4680
Acquisition Date	2009-02-25T18:25:49
Modification Date	2012-04-23T11:56:58
Spectrometer Frequency	175.97
Spectral Width	44642.9
Lowest Frequency	-2967.2
Nucleus	¹³ C
Acquired Size	65536
Spectral Size	131072

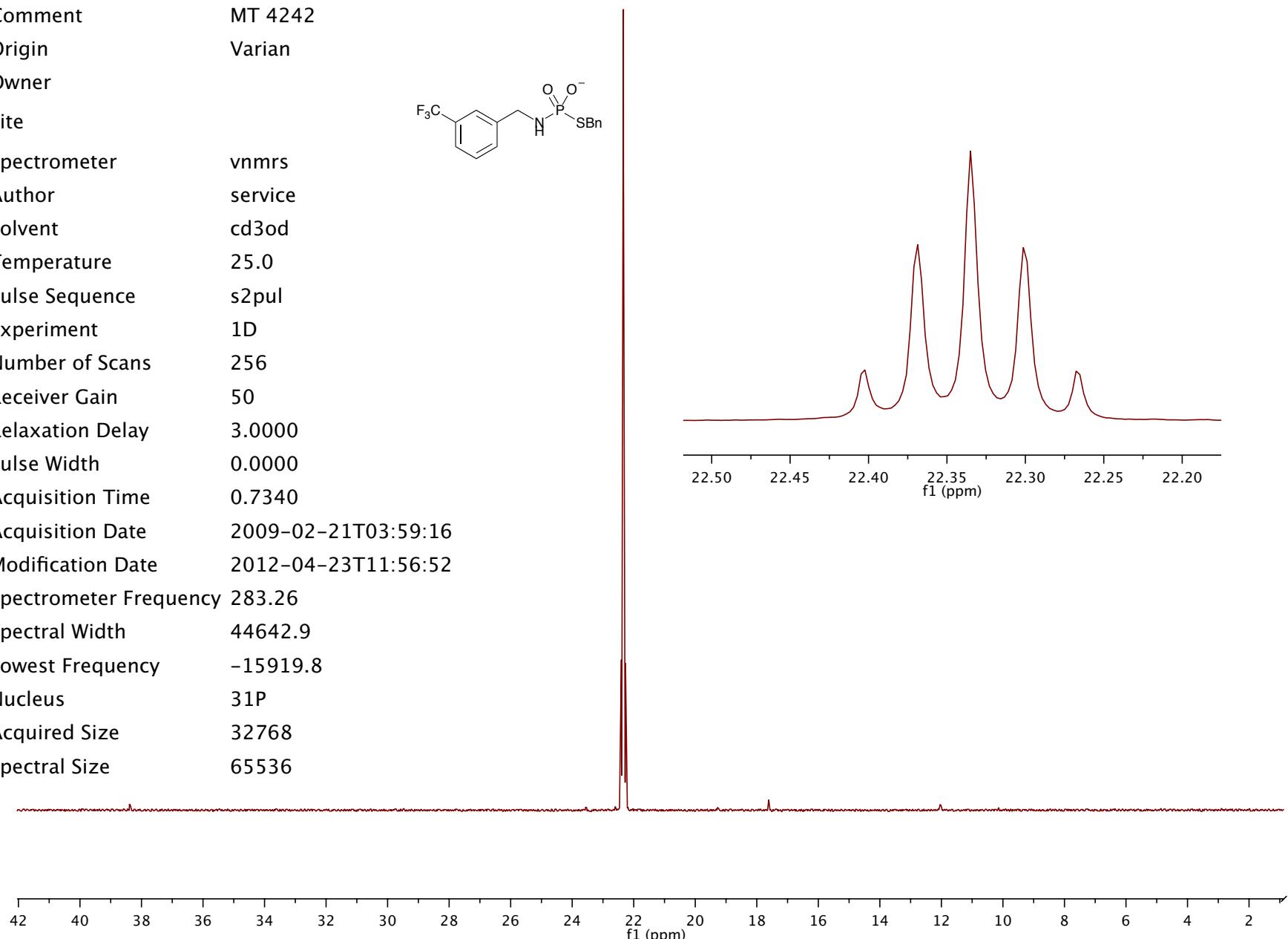


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Origin	Bruker BioSpin GmbH
Owner	Administrator
Site	
Spectrometer	av400
Author	
Solvent	MeOD
Temperature	293.2
Pulse Sequence	zgflqn
Experiment	1D
Number of Scans	16
Receiver Gain	813
Relaxation Delay	2.0000
Pulse Width	11.8000
Acquisition Time	0.8717
Acquisition Date	2009-05-11T13:05:00
Modification Date	2012-04-20T15:17:52
Spectrometer Frequency	376.39
Spectral Width	75188.0
Lowest Frequency	-71472.1
Nucleus	19F
Acquired Size	65536
Spectral Size	131072

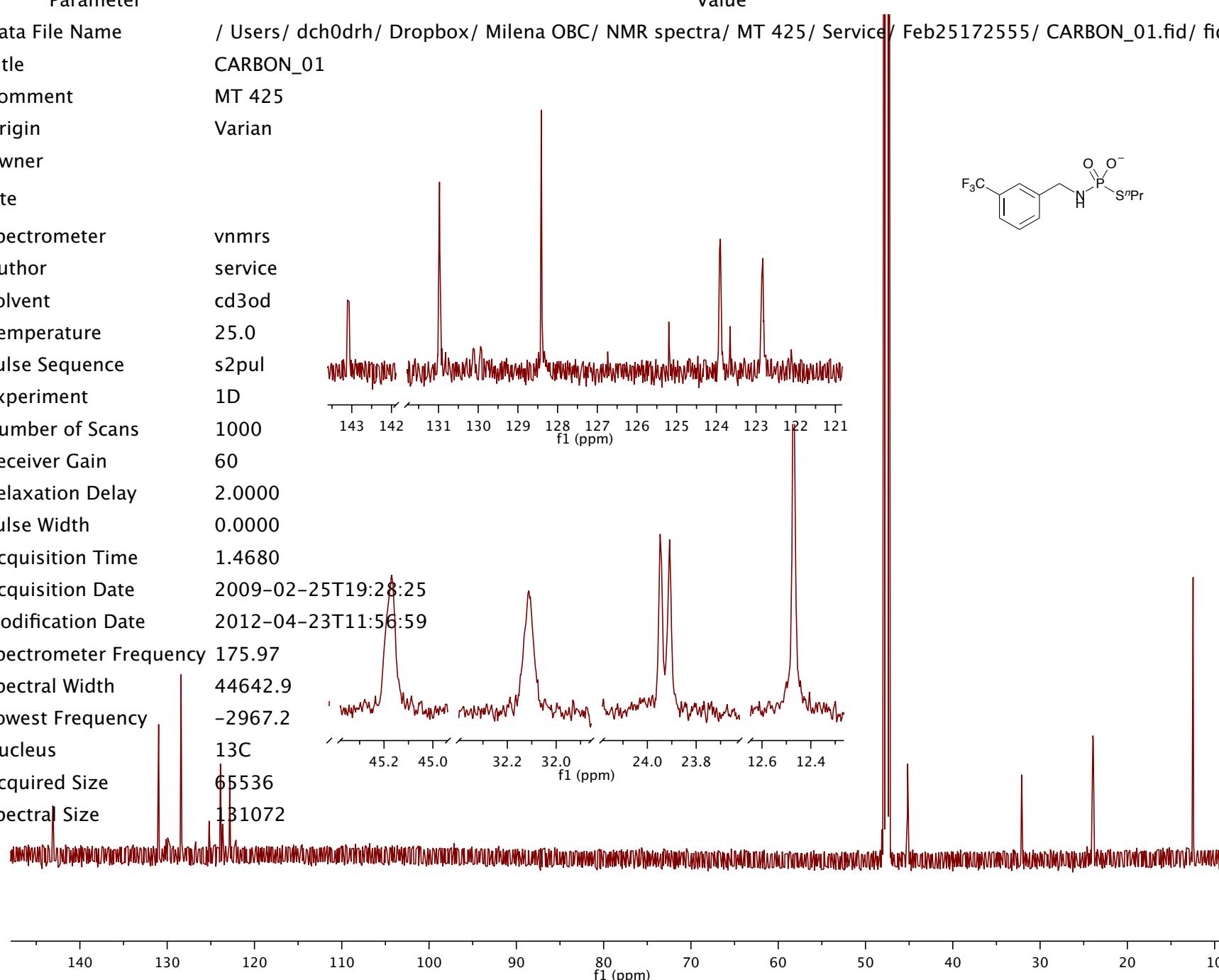




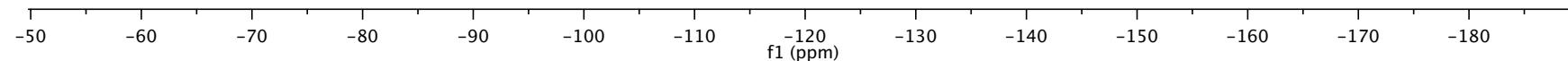
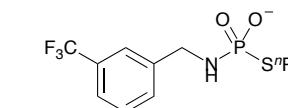
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Comment	MT 4242
Origin	Varian
Owner	
Site	
Spectrometer	vnmrs
Author	service
Solvent	cd3od
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	256
Receiver Gain	50
Relaxation Delay	3.0000
Pulse Width	0.0000
Acquisition Time	0.7340
Acquisition Date	2009-02-21T03:59:16
Modification Date	2012-04-23T11:56:52
Spectrometer Frequency	283.26
Spectral Width	44642.9
Lowest Frequency	-15919.8
Nucleus	³¹ P
Acquired Size	32768
Spectral Size	65536

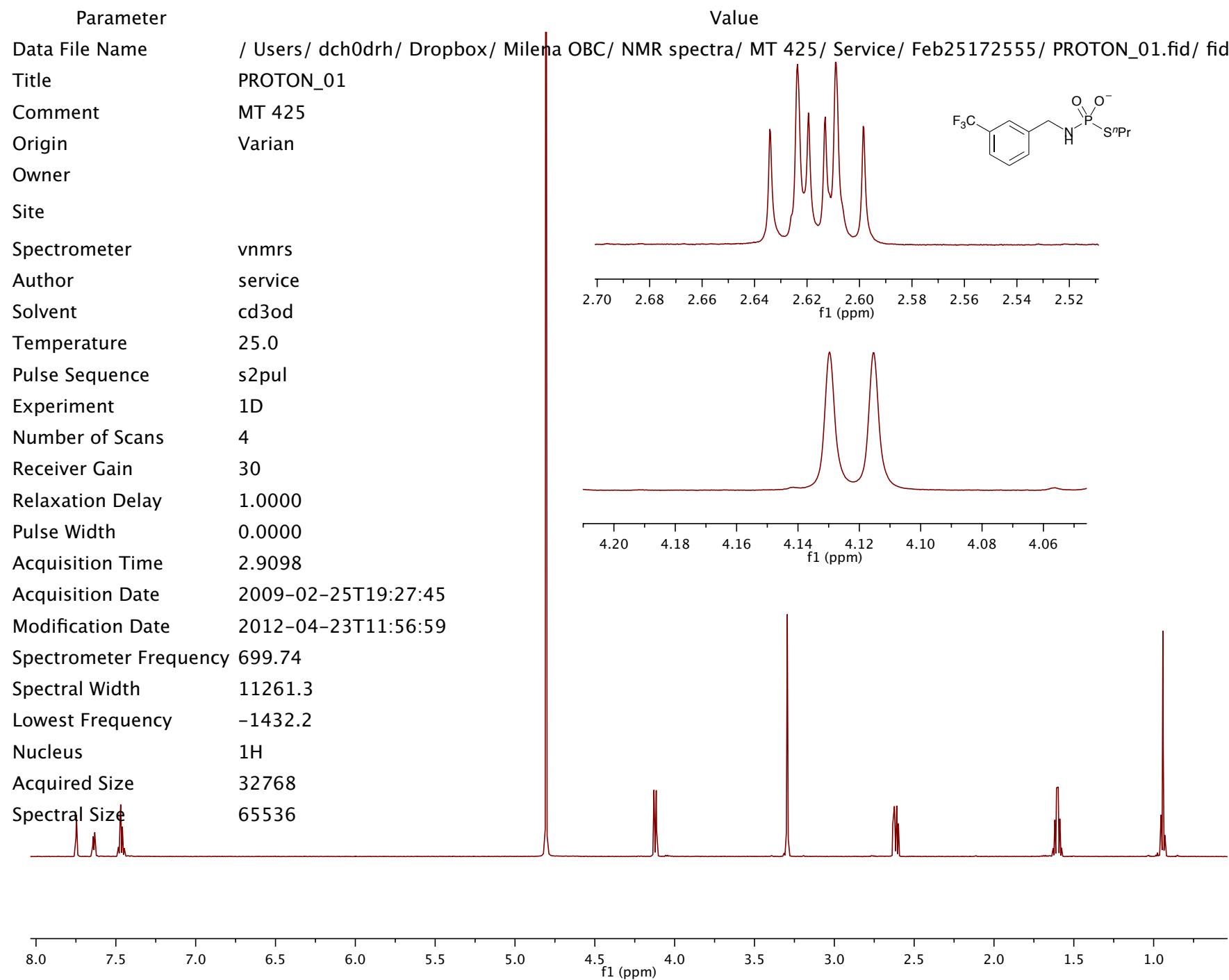


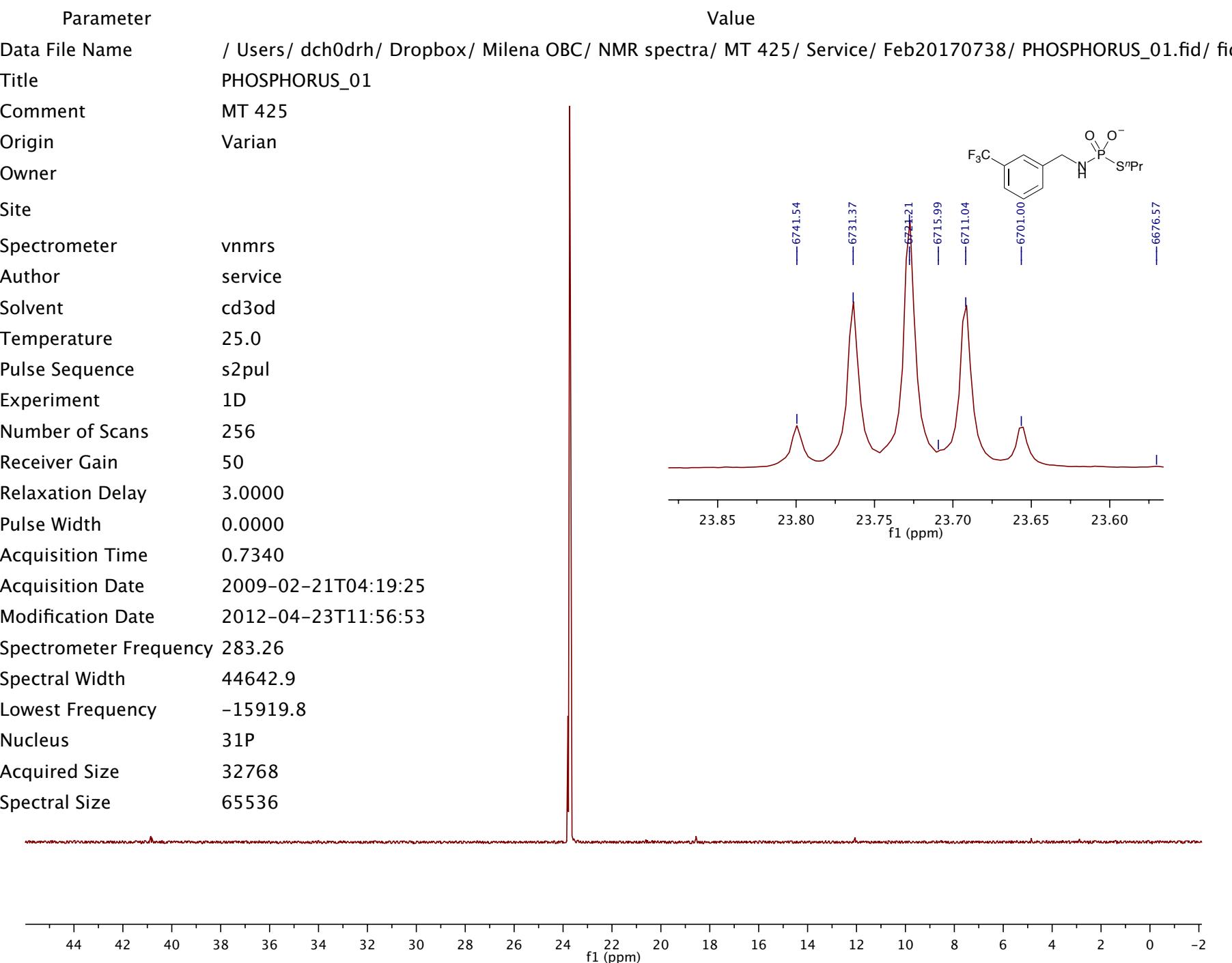
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Site	
Spectrometer	vnmrs
Author	service
Solvent	cd3od
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	1000
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.4680
Acquisition Date	2009-02-25T19:28:25
Modification Date	2012-04-23T11:56:59
Spectrometer Frequency	175.97
Spectral Width	44642.9
Lowest Frequency	-2967.2
Nucleus	¹³ C
Acquired Size	65536
Spectral Size	131072



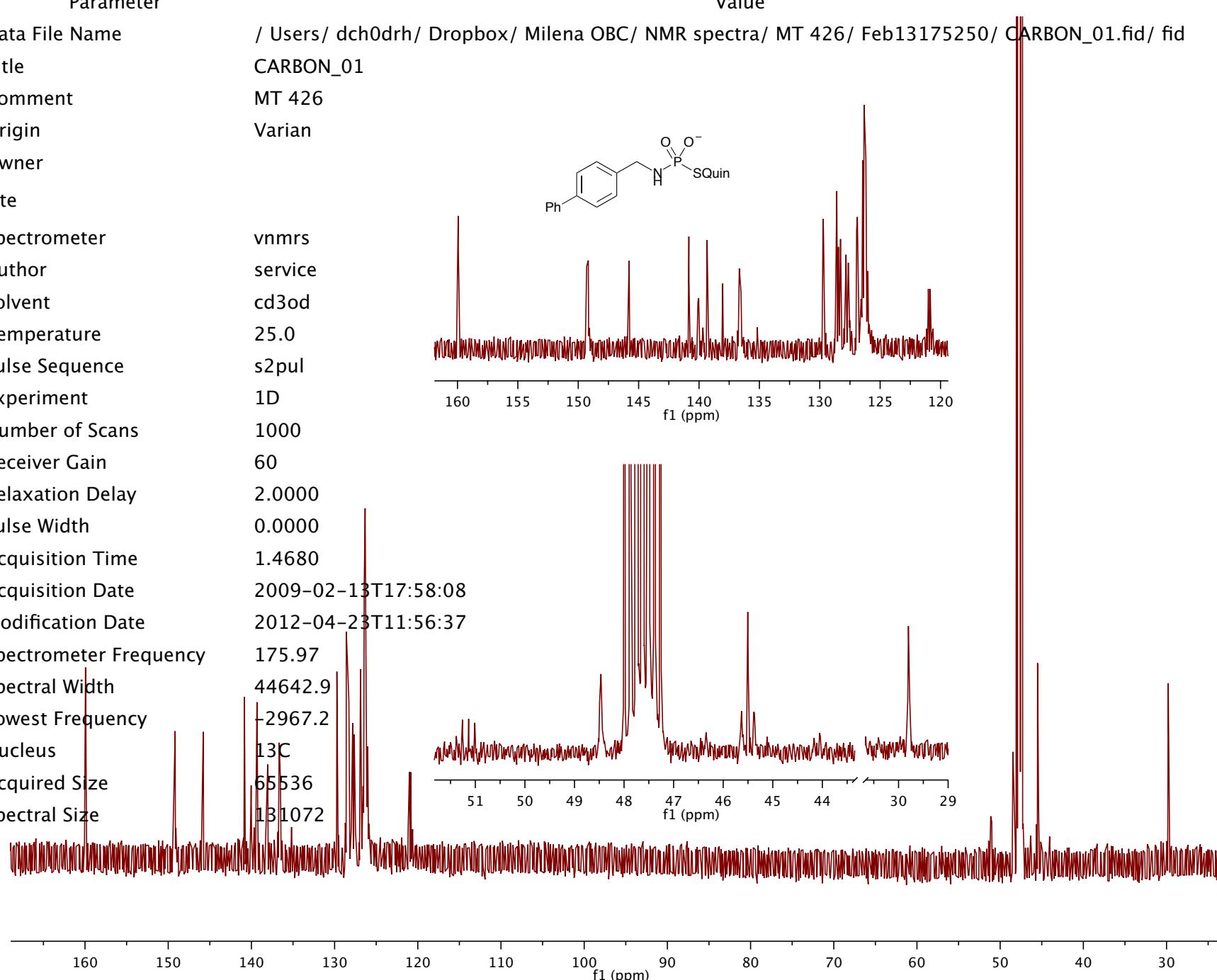
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Origin	Bruker BioSpin GmbH
Owner	Administrator
Site	
Spectrometer	av400
Author	
Solvent	MeOD
Temperature	293.3
Pulse Sequence	zgflqn
Experiment	1D
Number of Scans	16
Receiver Gain	813
Relaxation Delay	2.0000
Pulse Width	11.8000
Acquisition Time	0.8717
Acquisition Date	2009-05-11T13:12:00
Modification Date	2012-04-20T15:17:52
Spectrometer Frequency	376.39
Spectral Width	75188.0
Lowest Frequency	-71472.1
Nucleus	19F
Acquired Size	65536
Spectral Size	131072

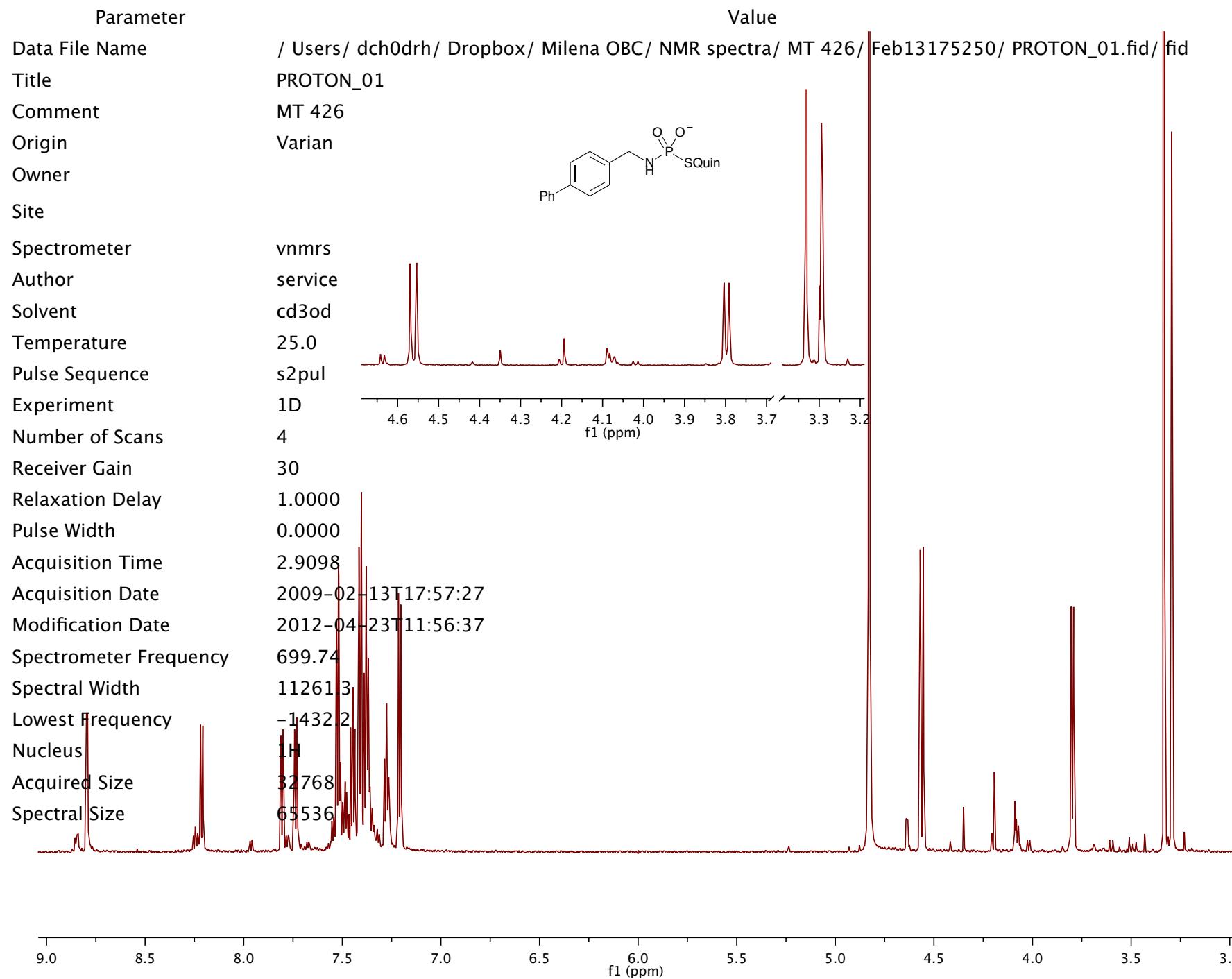


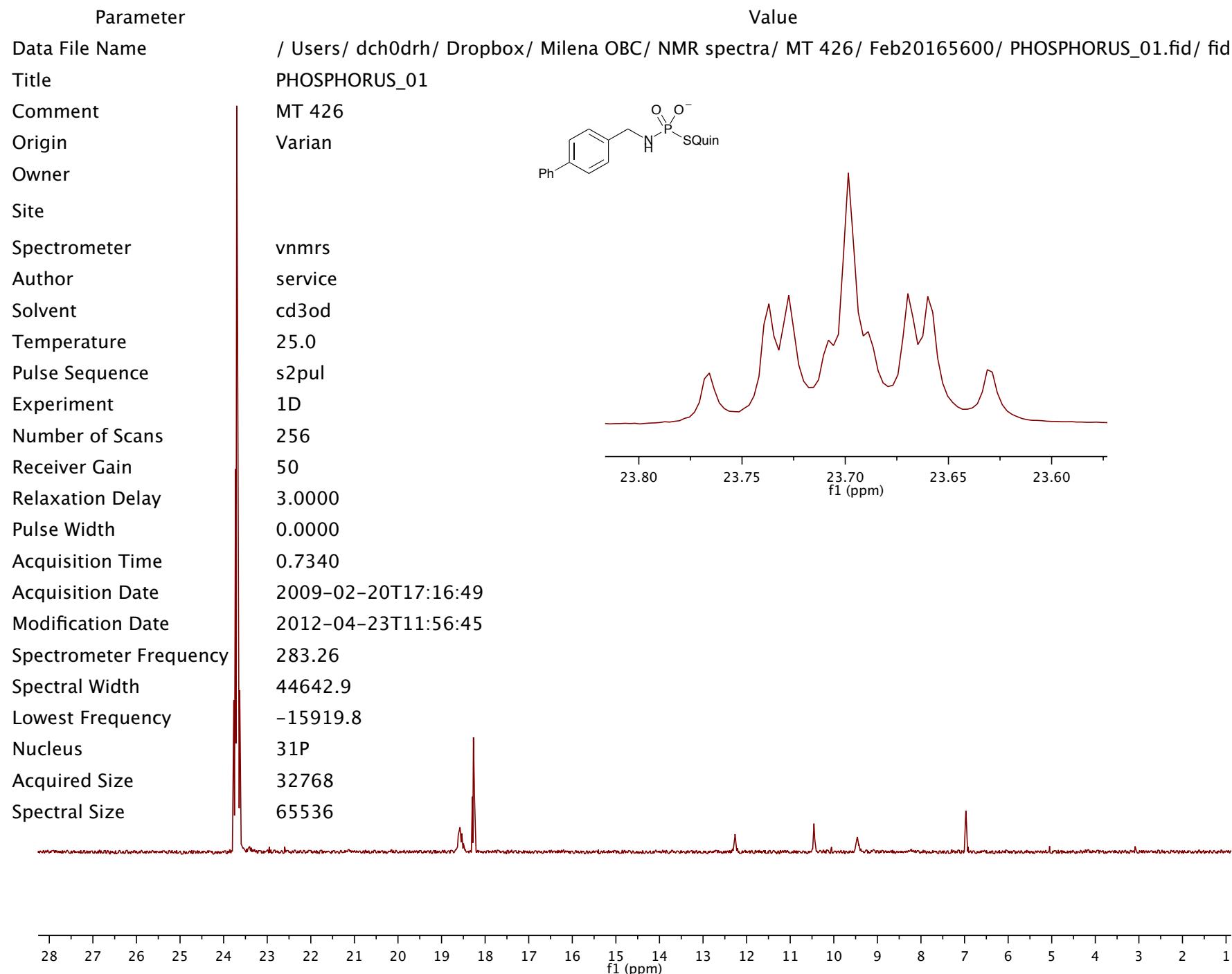


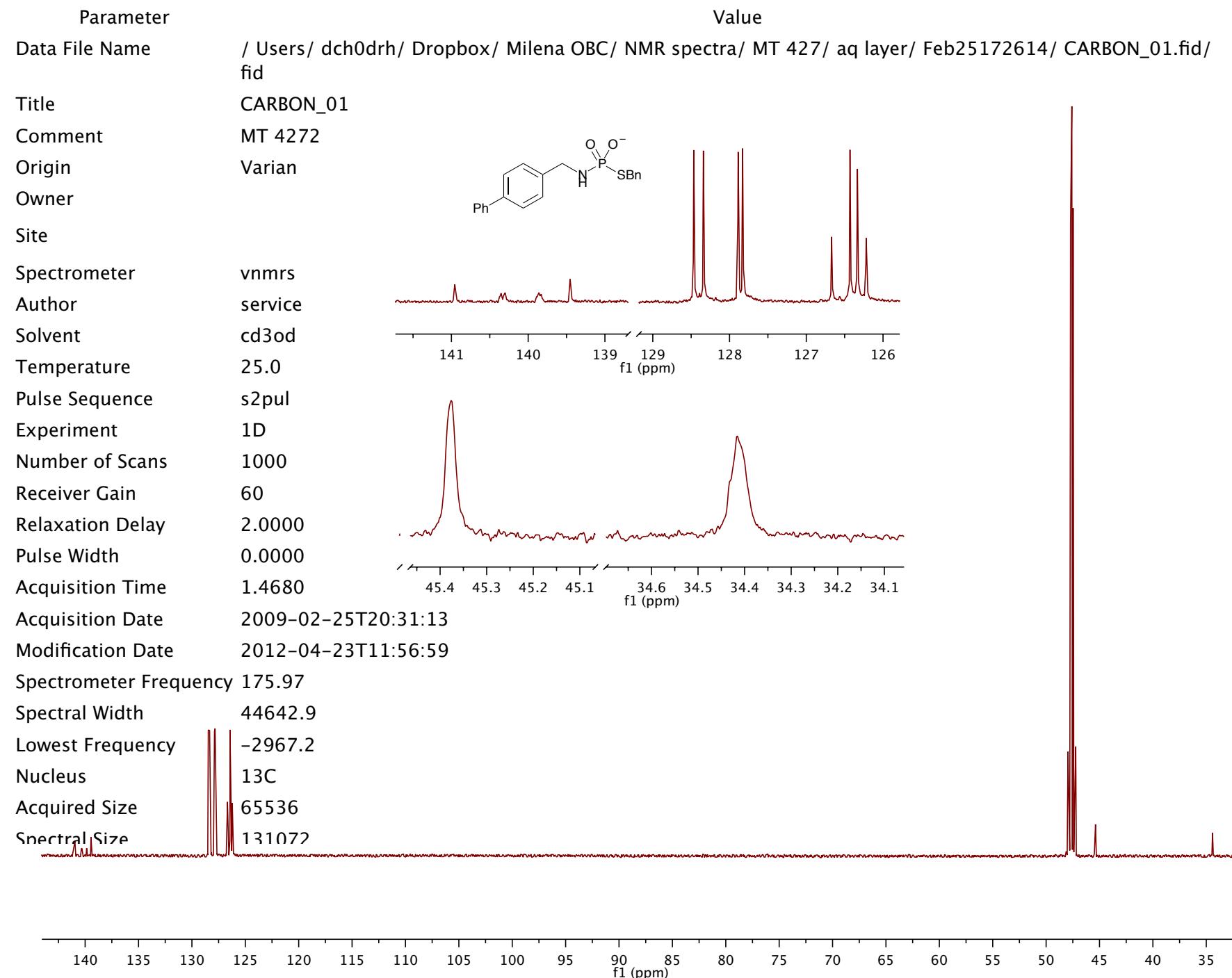


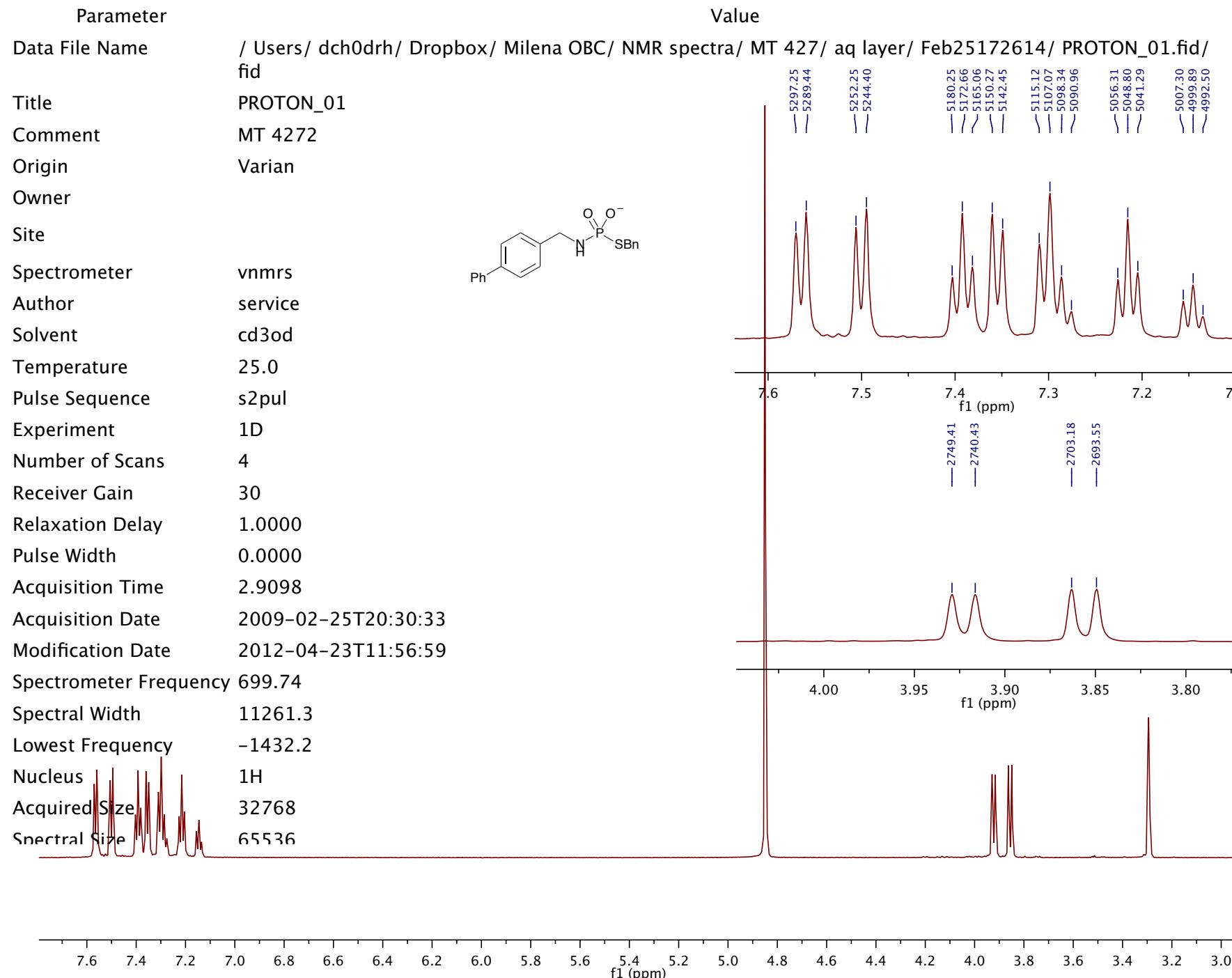
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Spectrometer	vnmrs
Author	service
Solvent	cd3od
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	1000
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.4680
Acquisition Date	2009-02-13T17:58:08
Modification Date	2012-04-23T11:56:37
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Nucleus	¹³ C
Acquired Size	65536
Spectral Size	131072







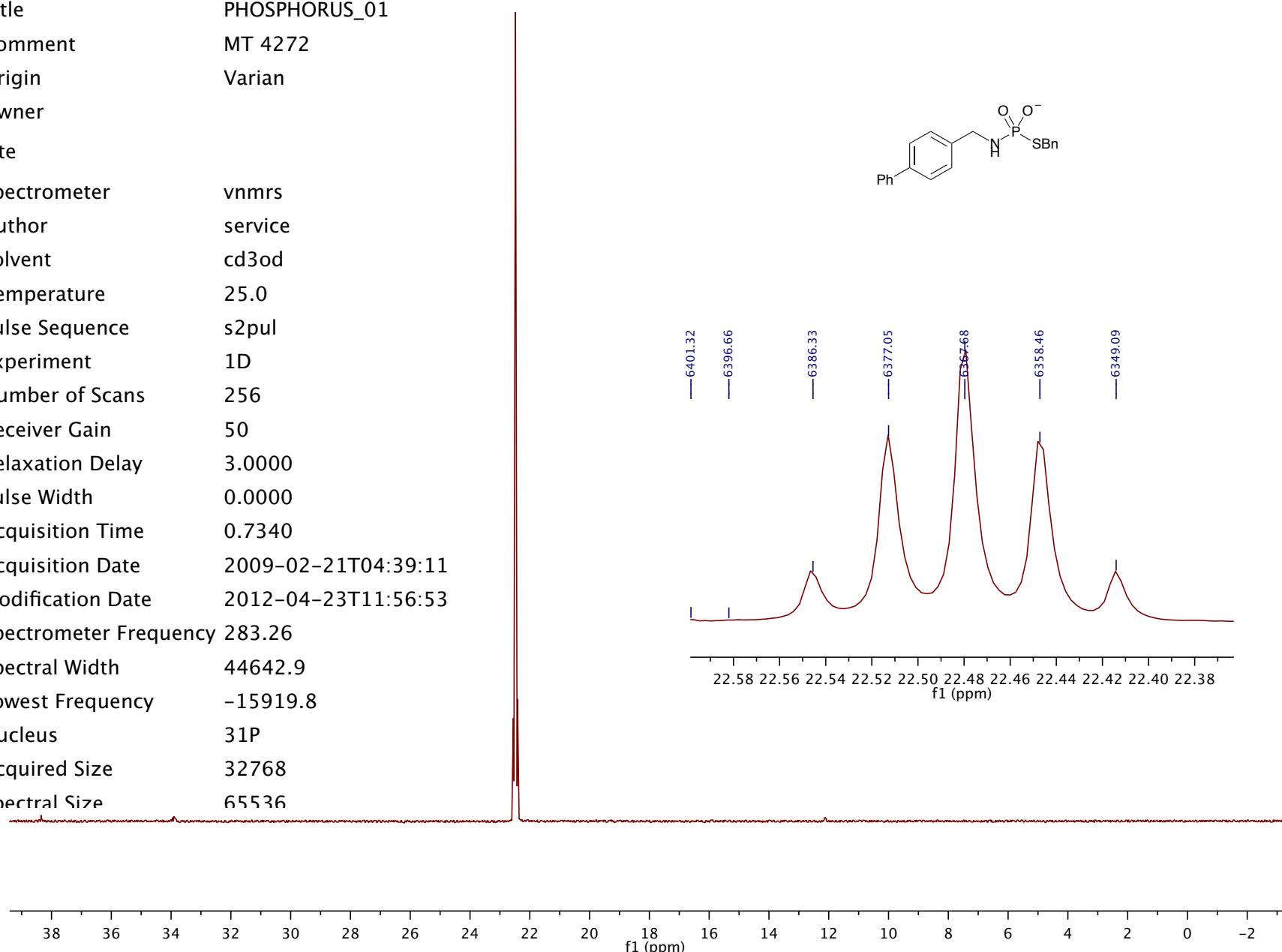


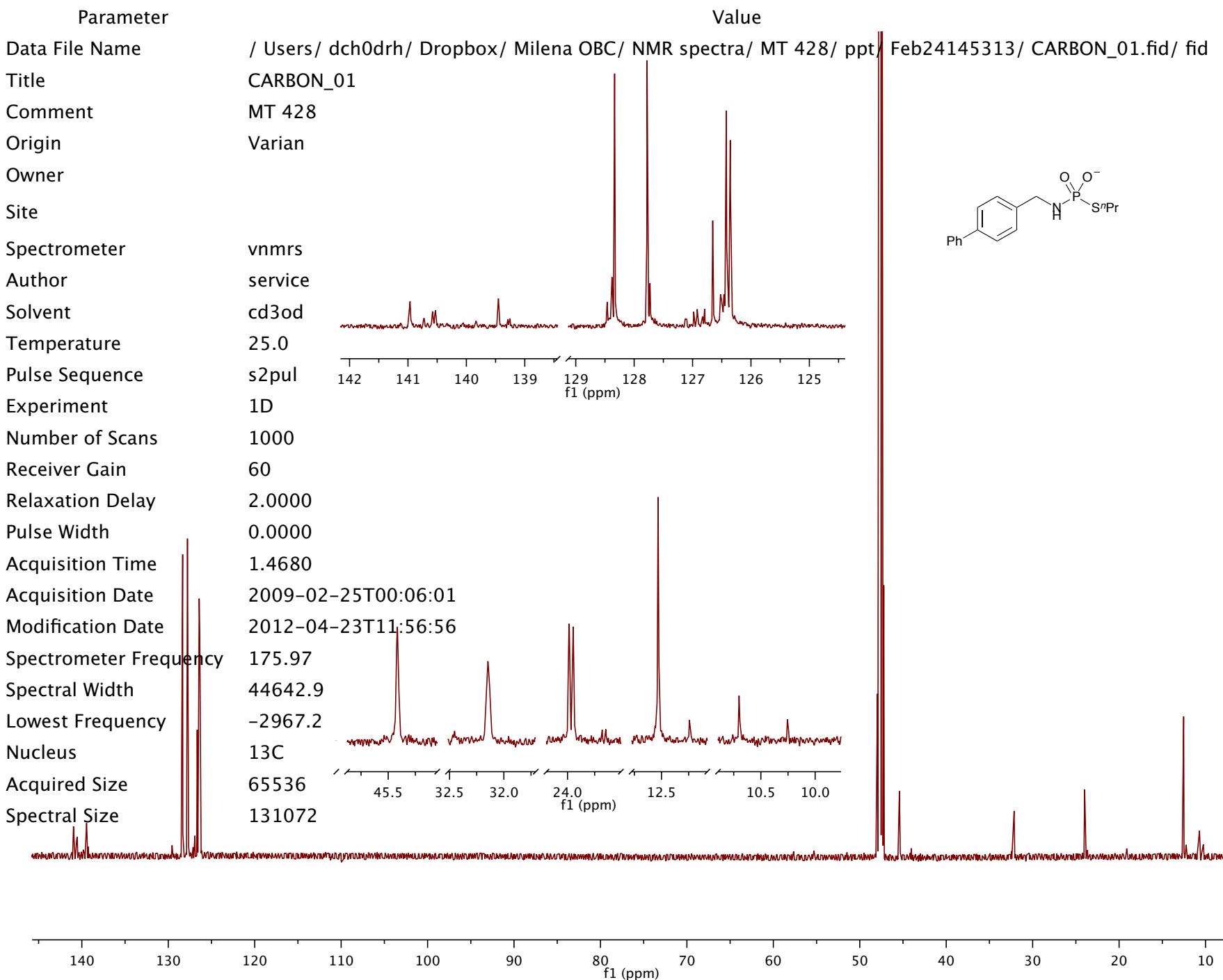


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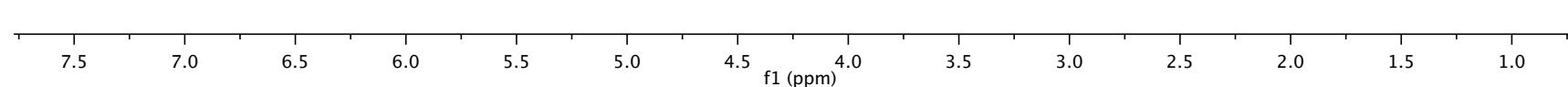
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Owner	
Site	
Spectrometer	vnmrs
Author	service
Solvent	cd3od
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	256
Receiver Gain	50
Relaxation Delay	3.0000
Pulse Width	0.0000
Acquisition Time	0.7340
Acquisition Date	2009-02-21T04:39:11
Modification Date	2012-04-23T11:56:53
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Spectral Width	44642.9
Lowest Frequency	-15919.8
Nucleus	³¹ P
Acquired Size	32768
Spectral Size	65536

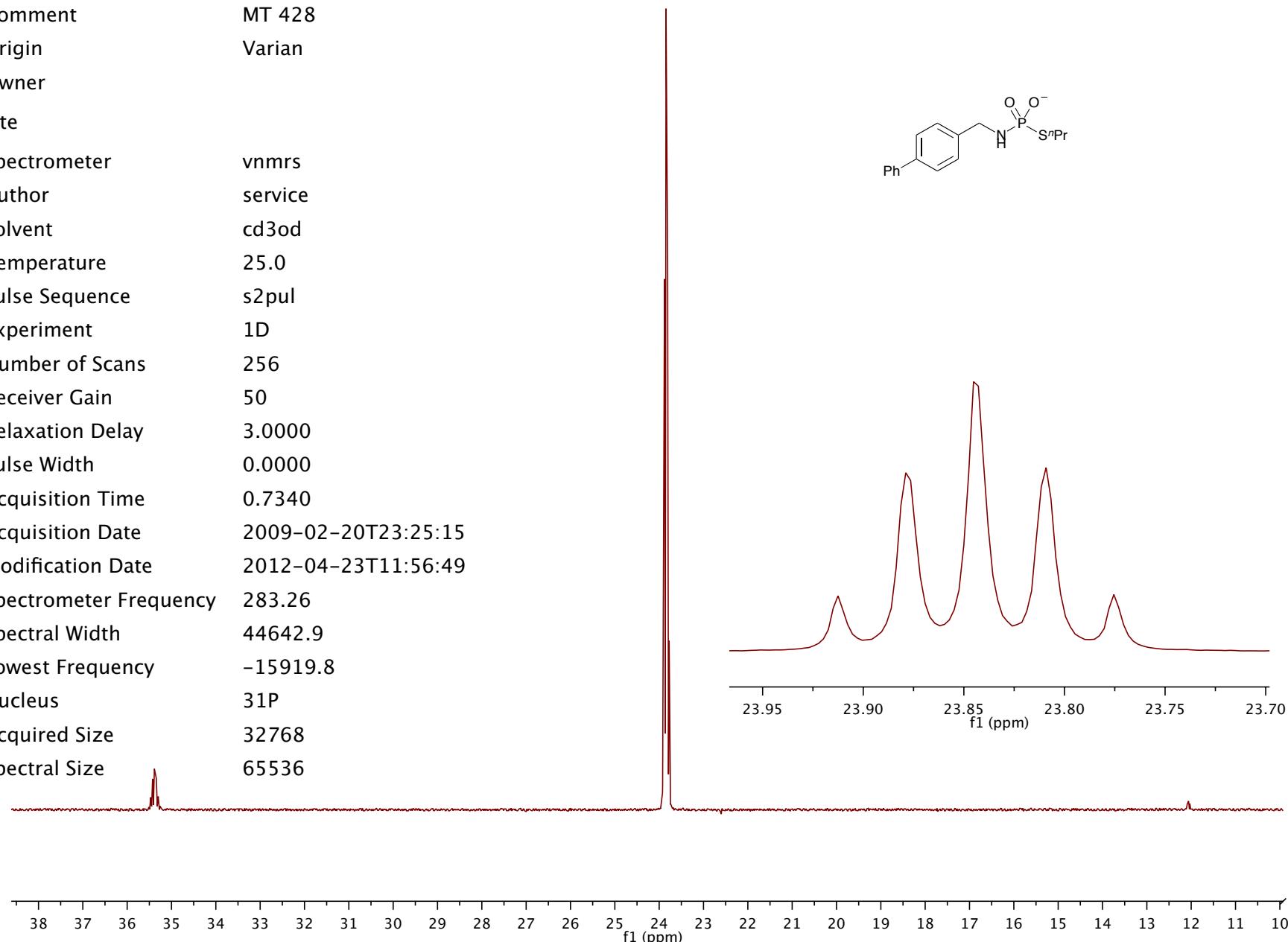


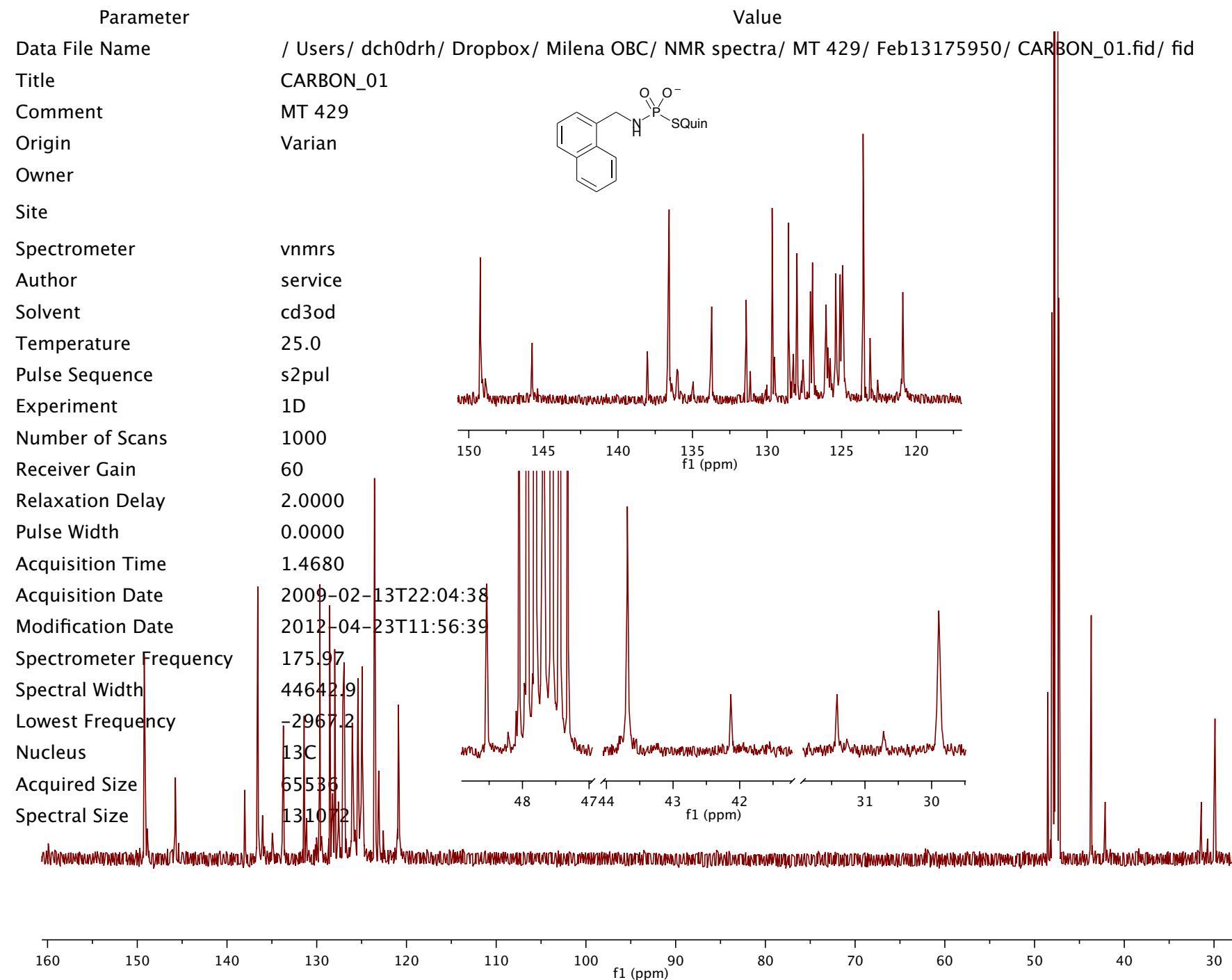


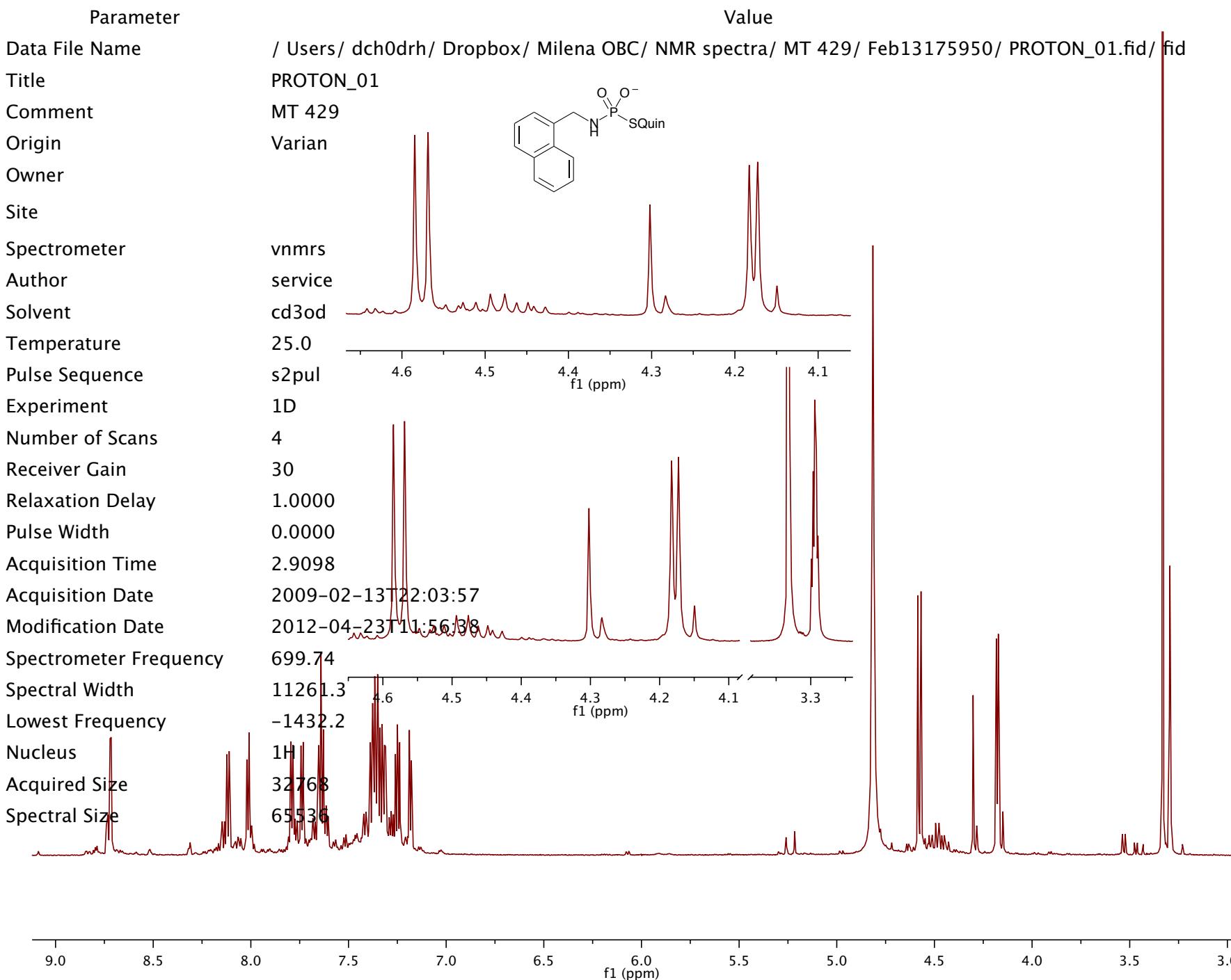
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Origin	Varian
Owner	
Site	
Spectrometer	vnmrs
Author	service
Solvent	cd3od
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	4
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	2.9098
Acquisition Date	2009-02-25T00:05:20
Modification Date	2012-04-23T11:56:56
Spectrometer Frequency	699.74
Spectral Width	11261.3
Lowest Frequency	-1432.2
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

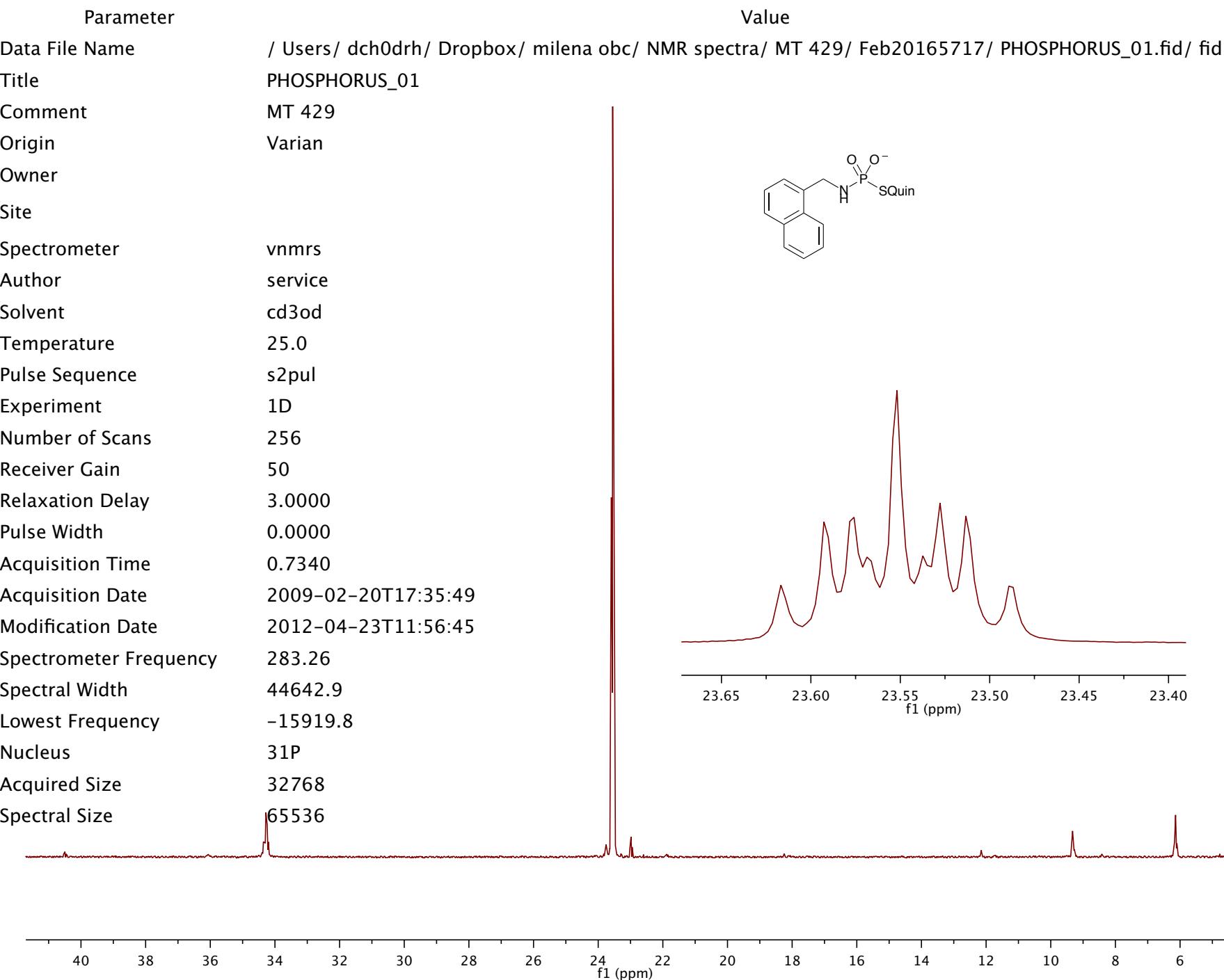


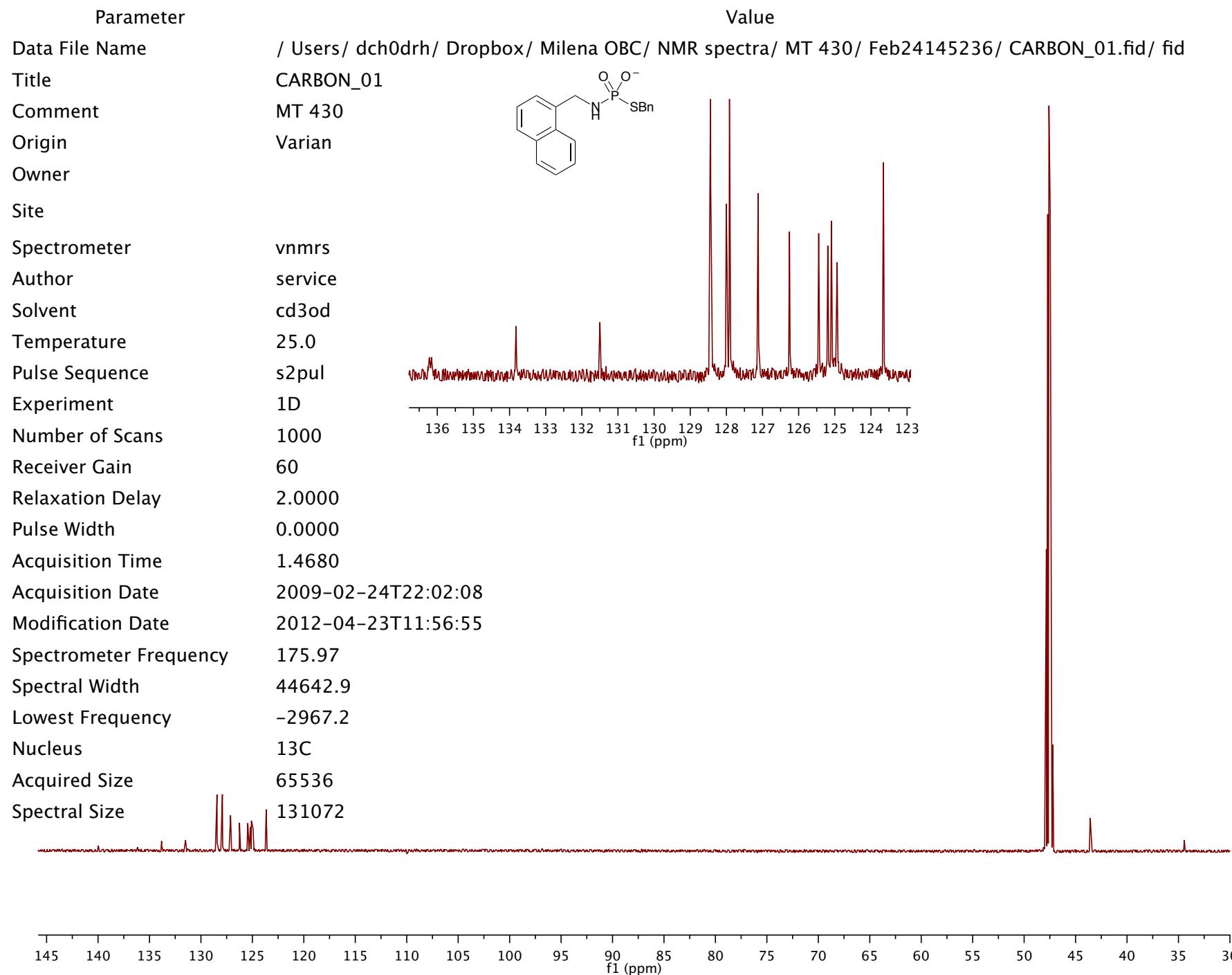
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Owner	
Site	
Spectrometer	vnmrs
Author	service
Solvent	cd3od
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	256
Receiver Gain	50
Relaxation Delay	3.0000
Pulse Width	0.0000
Acquisition Time	0.7340
Acquisition Date	2009-02-20T23:25:15
Modification Date	2012-04-23T11:56:49
Spectrometer Frequency	283.26
Spectral Width	44642.9
Lowest Frequency	-15919.8
Nucleus	³¹ P
Acquired Size	32768
Spectral Size	65536

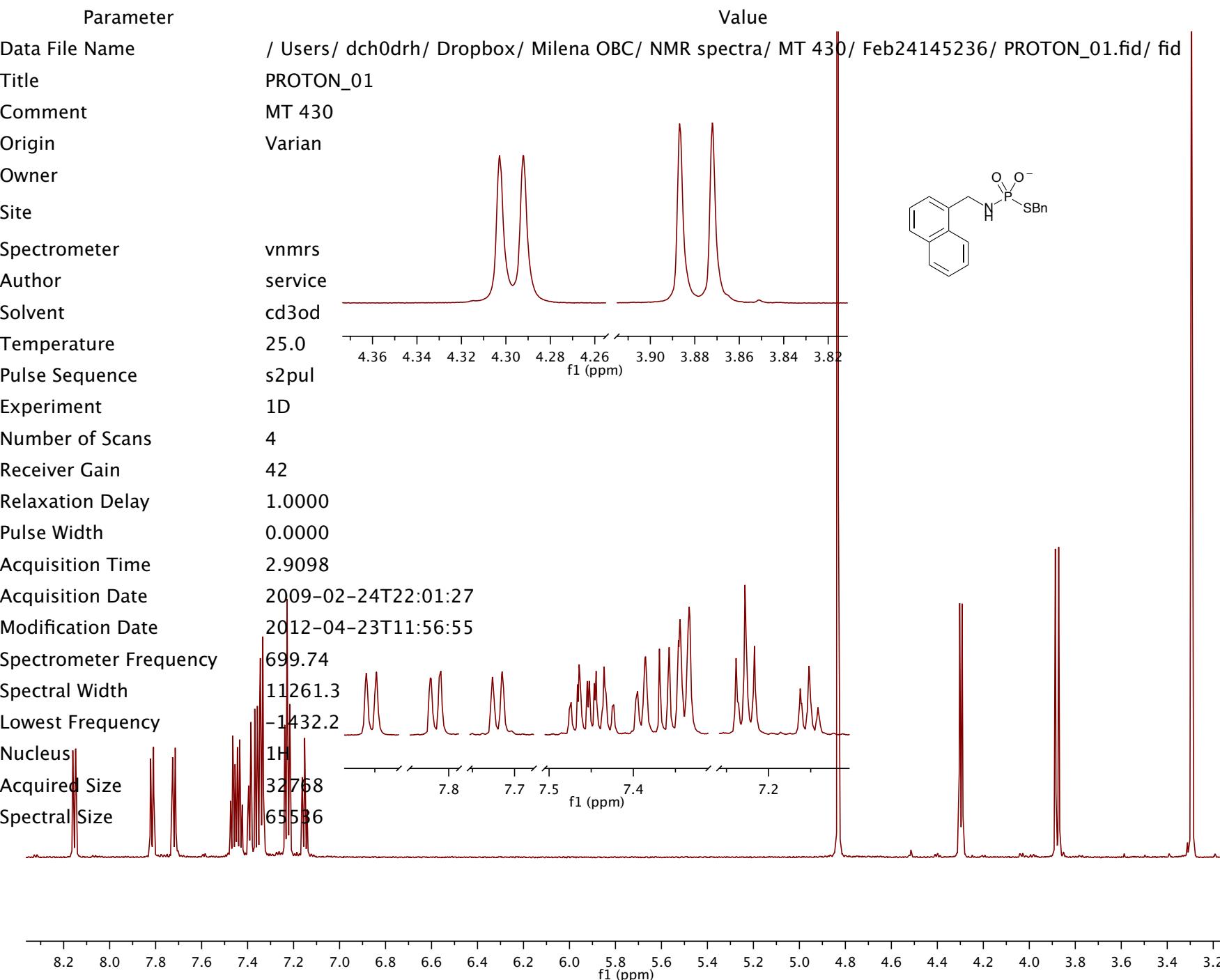




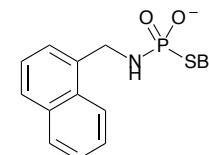
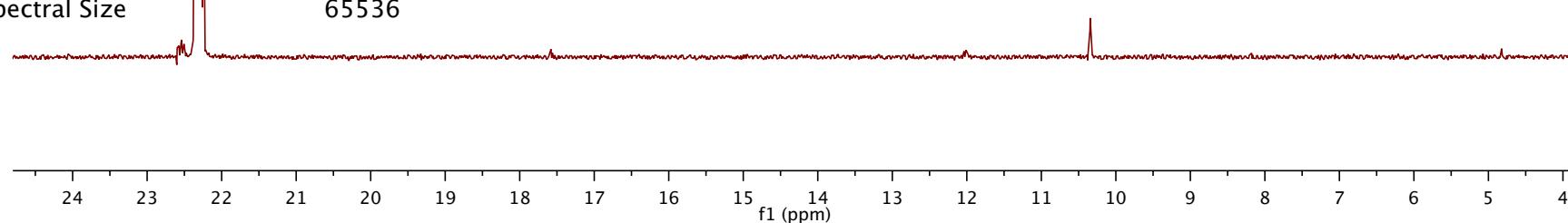


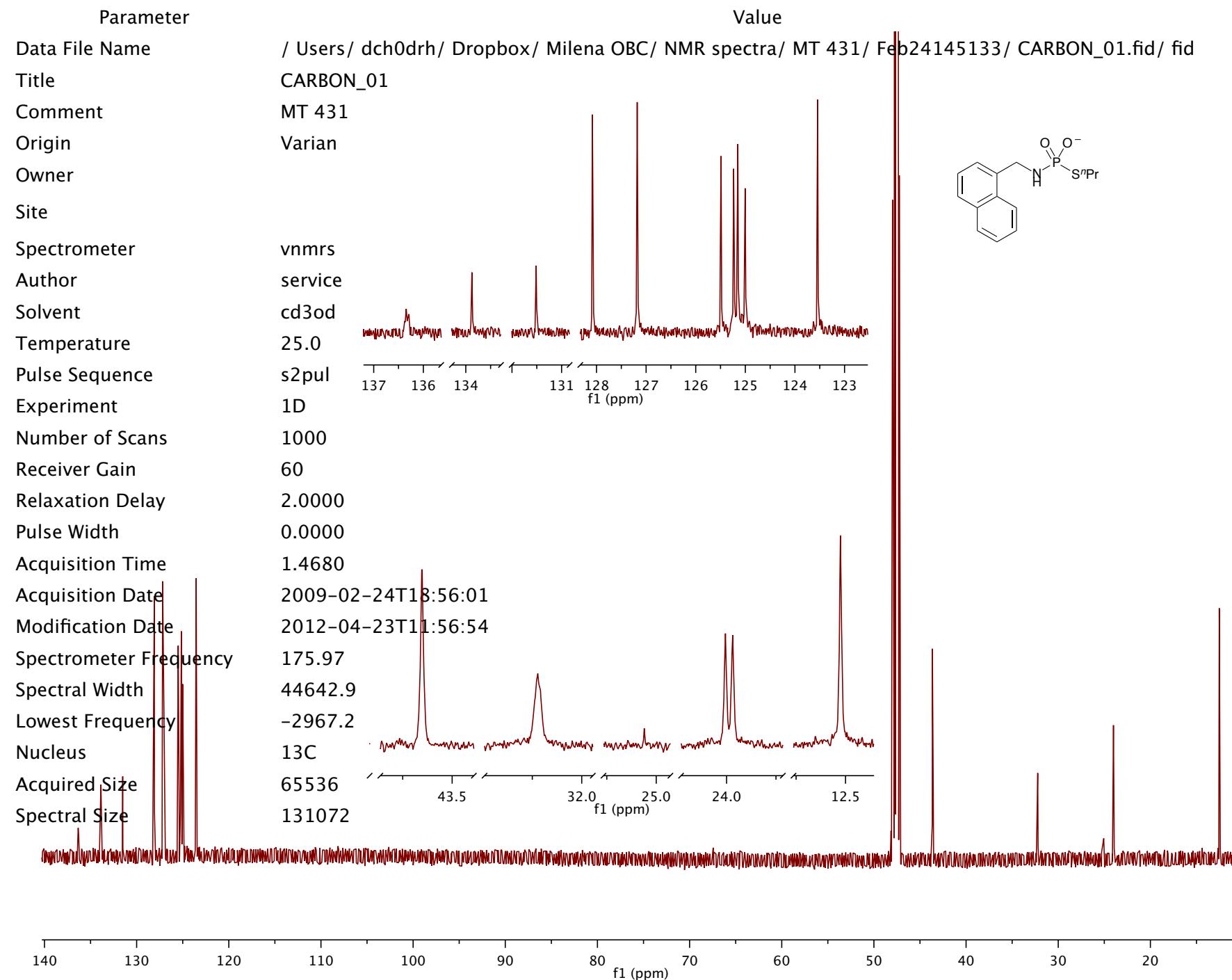


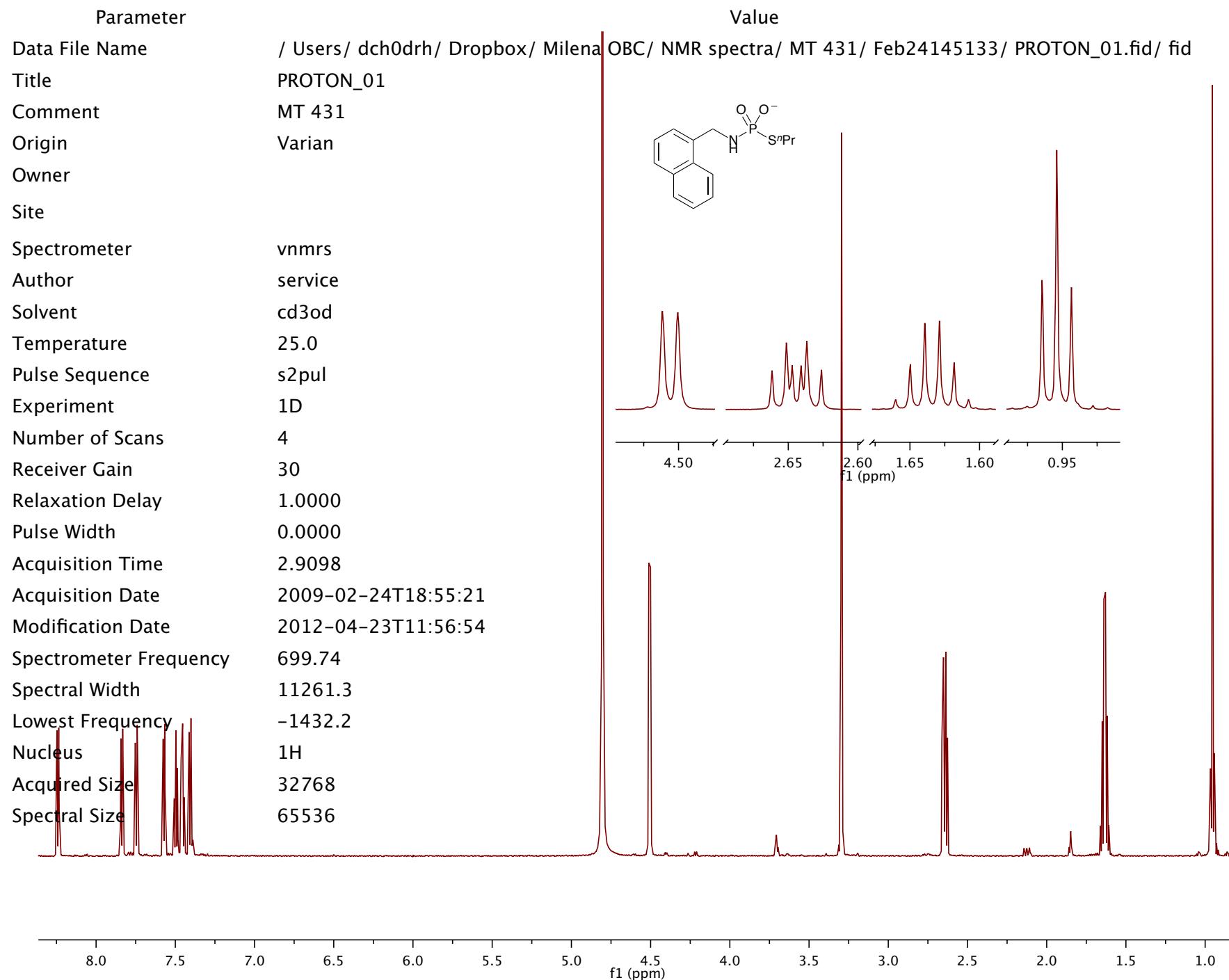




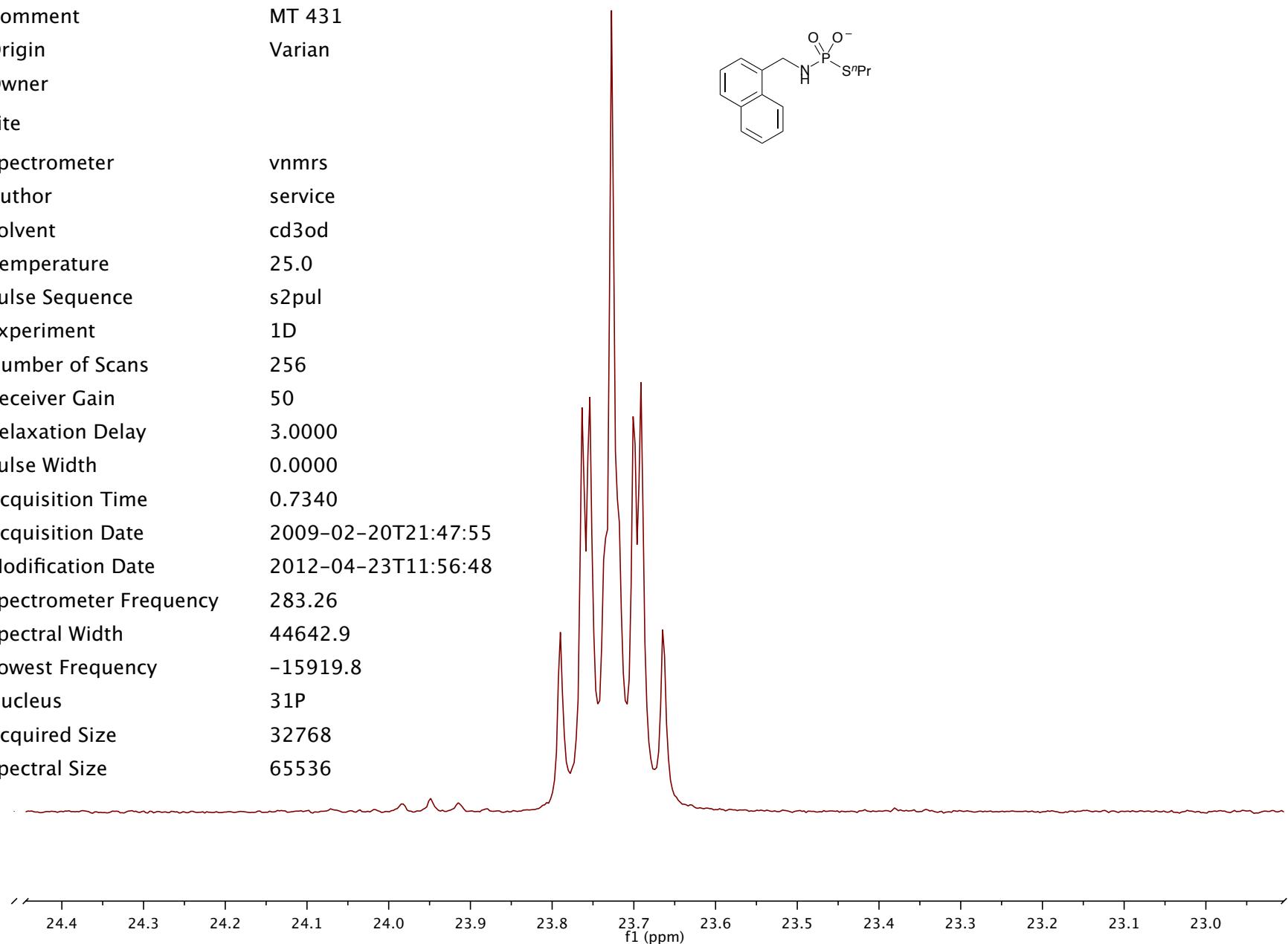
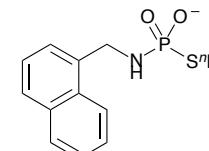
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Site	
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Author	service
Solvent	cd3od
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	256
Receiver Gain	50
Relaxation Delay	3.0000
Pulse Width	0.0000
Acquisition Time	0.7340
Acquisition Date	2009-02-20T22:46:00
Modification Date	2012-04-23T11:56:48
Spectrometer Frequency	283.26
Spectral Width	44642.9
Lowest Frequency	-15919.8
Nucleus	31P
Acquired Size	32768
Spectral Size	65536

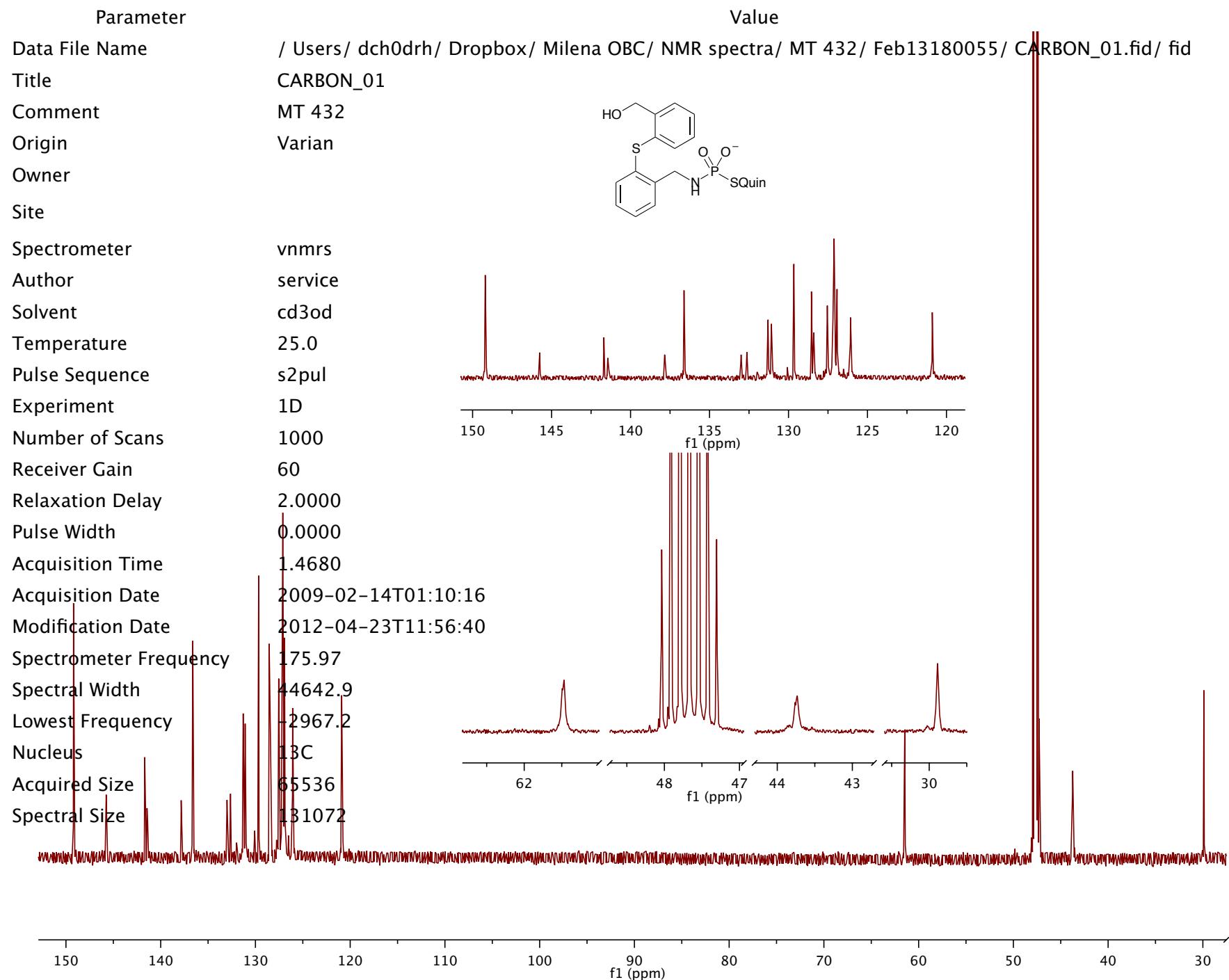


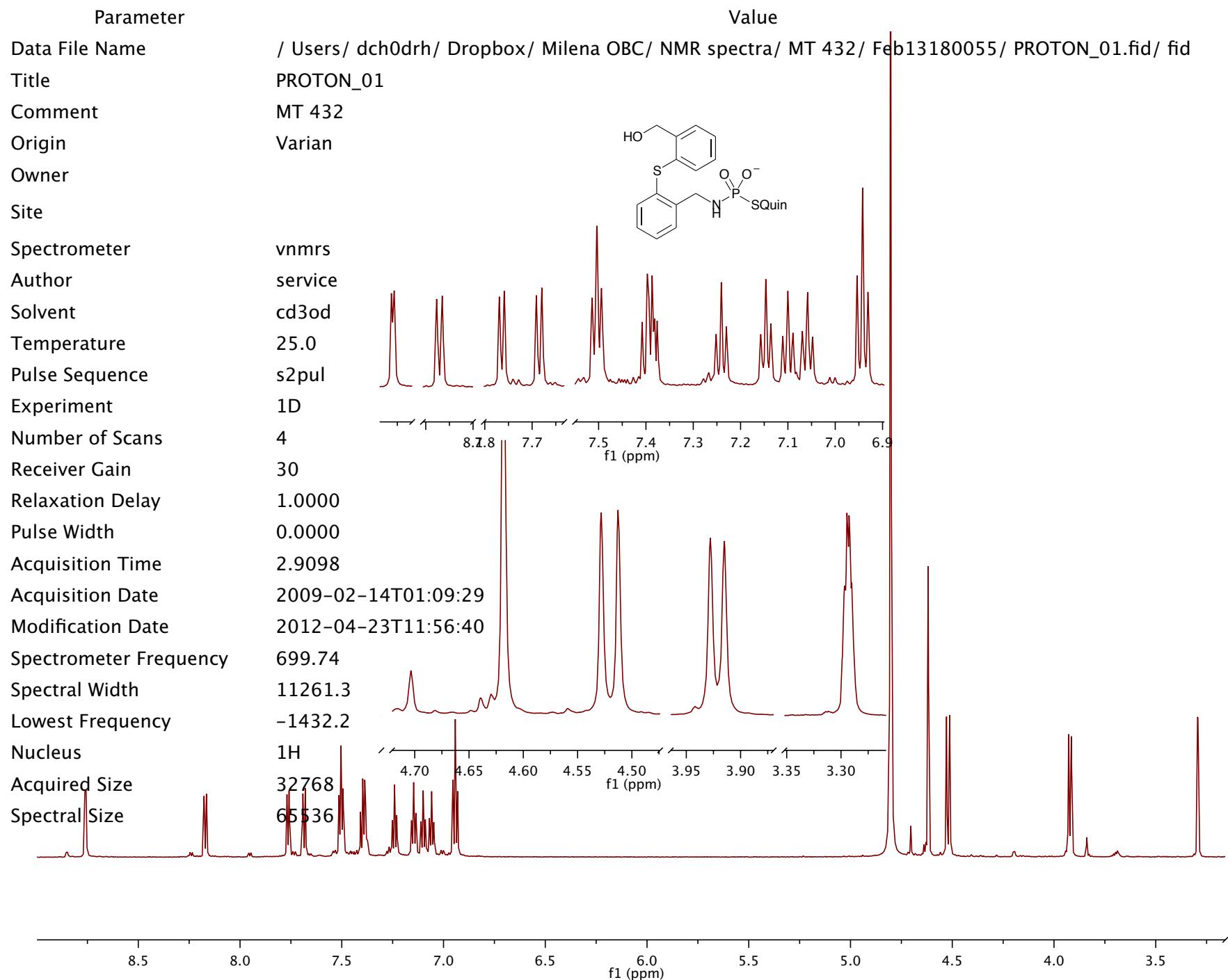




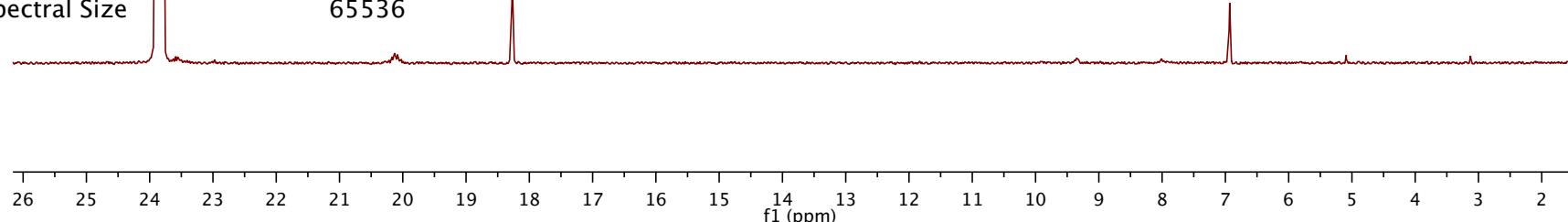
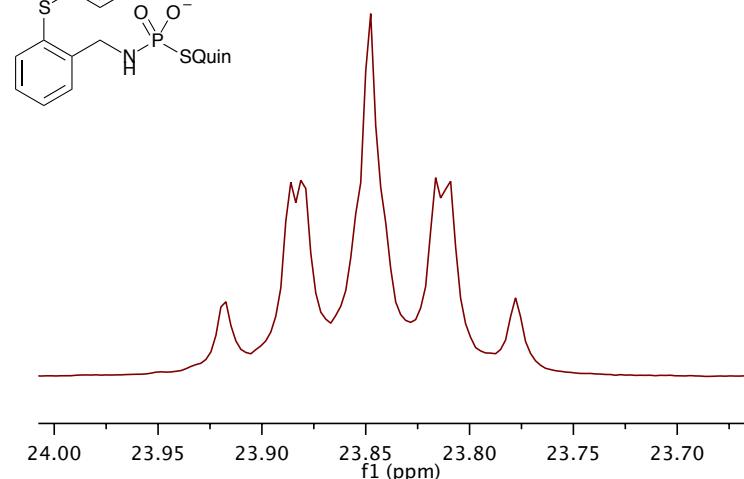
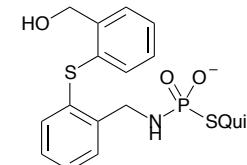
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Site	
Spectrometer	vnmrs
Author	service
Solvent	cd3od
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	256
Receiver Gain	50
Relaxation Delay	3.0000
Pulse Width	0.0000
Acquisition Time	0.7340
Acquisition Date	2009-02-20T21:47:55
Modification Date	2012-04-23T11:56:48
Spectrometer Frequency	283.26
Spectral Width	44642.9
Lowest Frequency	-15919.8
Nucleus	³¹ P
Acquired Size	32768
Spectral Size	65536

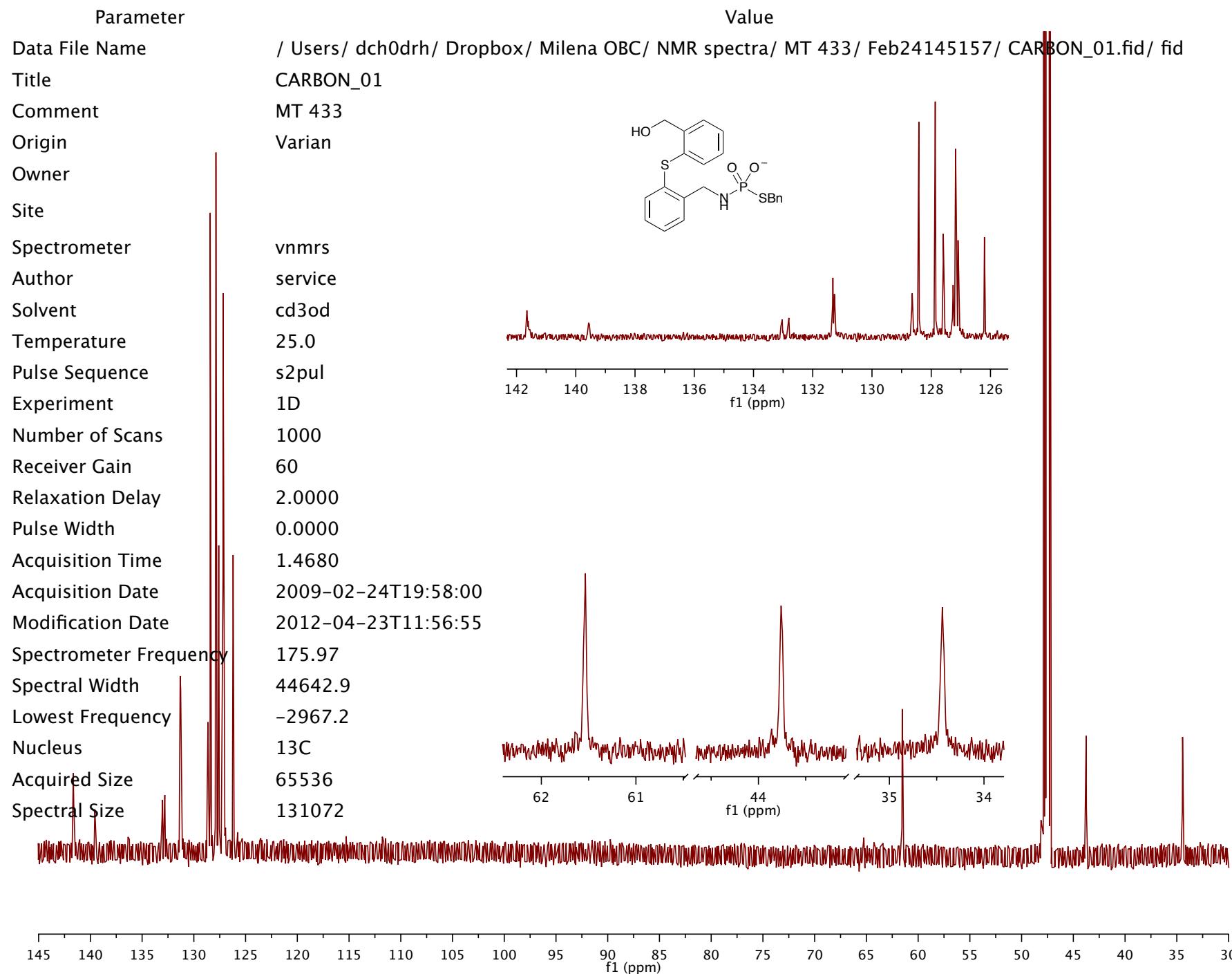




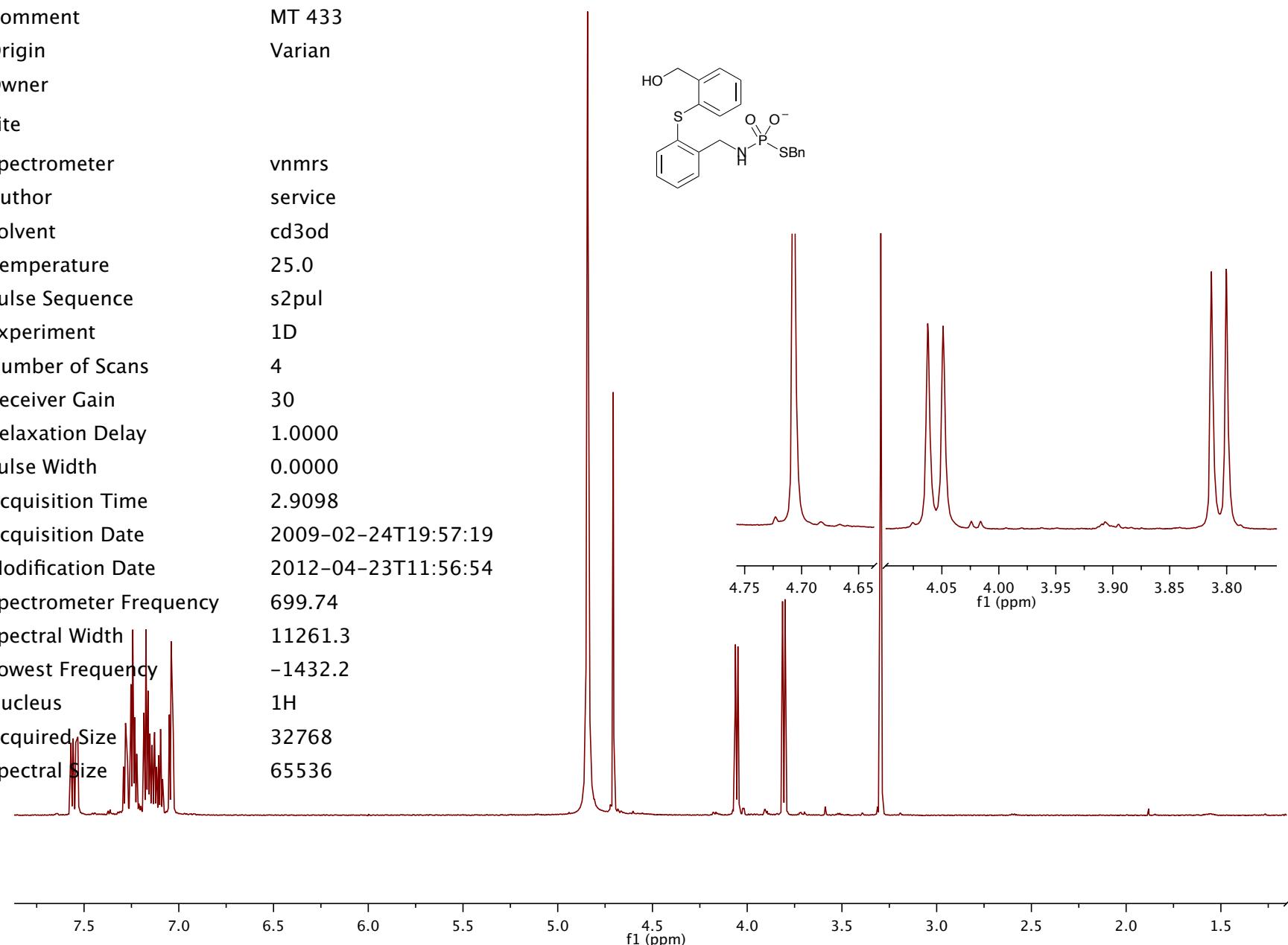


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Spectrometer	vnmrs
Author	service
Solvent	cd3od
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	256
Receiver Gain	50
Relaxation Delay	3.0000
Pulse Width	0.0000
Acquisition Time	0.7340
Acquisition Date	2009-02-20T17:54:48
Modification Date	2012-04-23T11:56:45
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Spectral Width	44642.9
Lowest Frequency	-15919.8
Nucleus	³¹ P
Acquired Size	32768
Spectral Size	65536

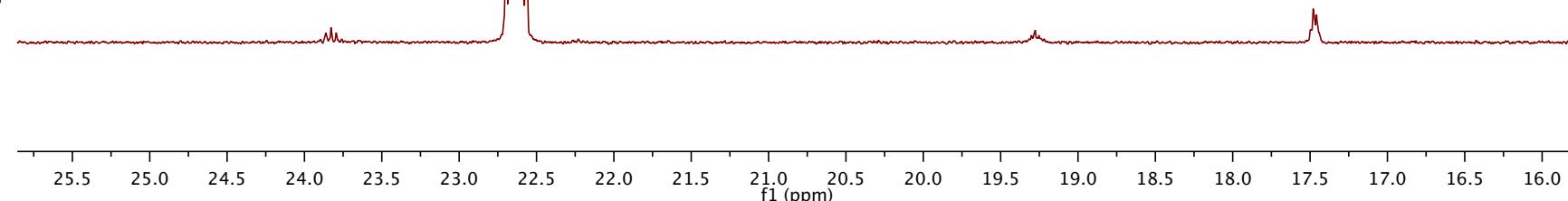


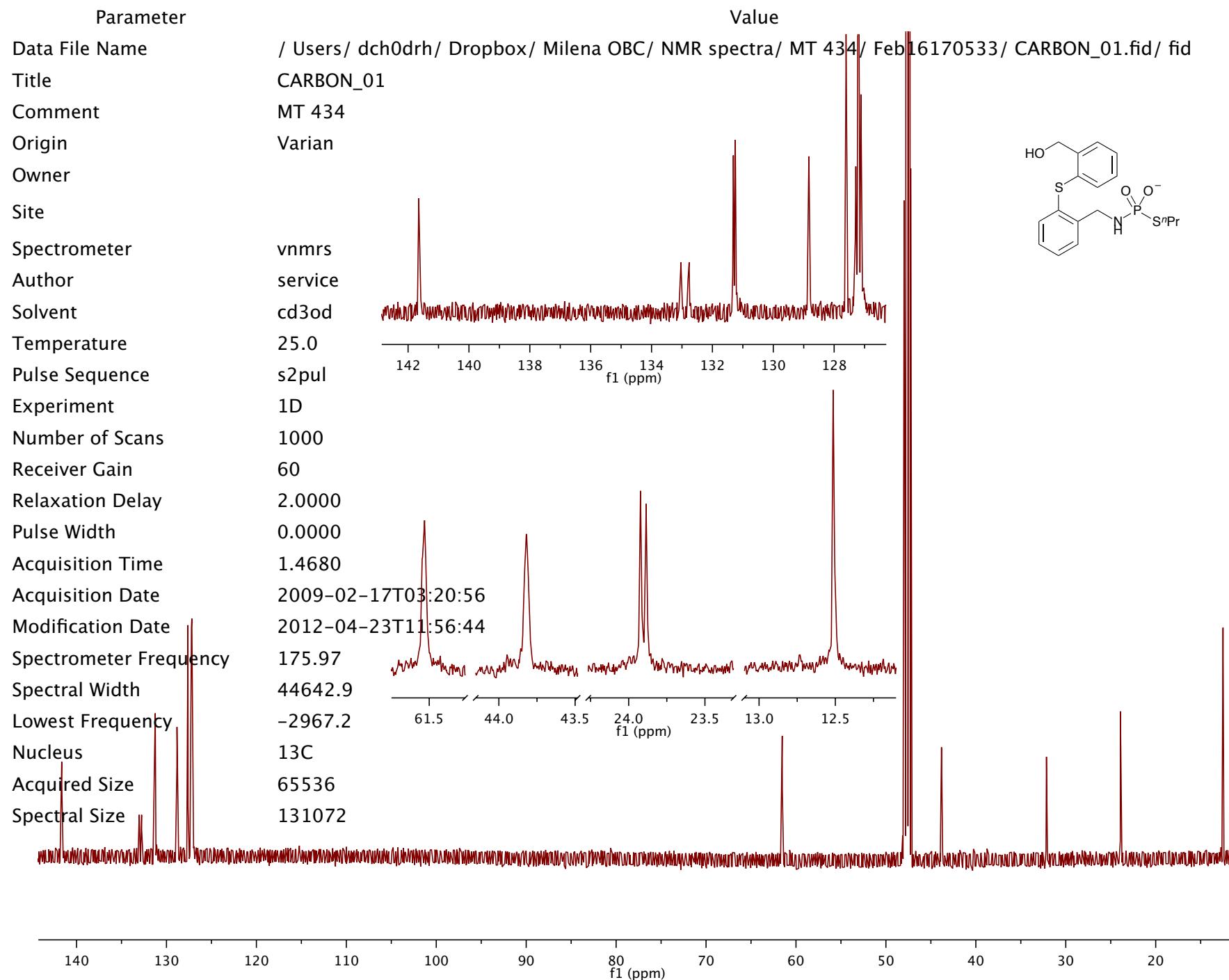


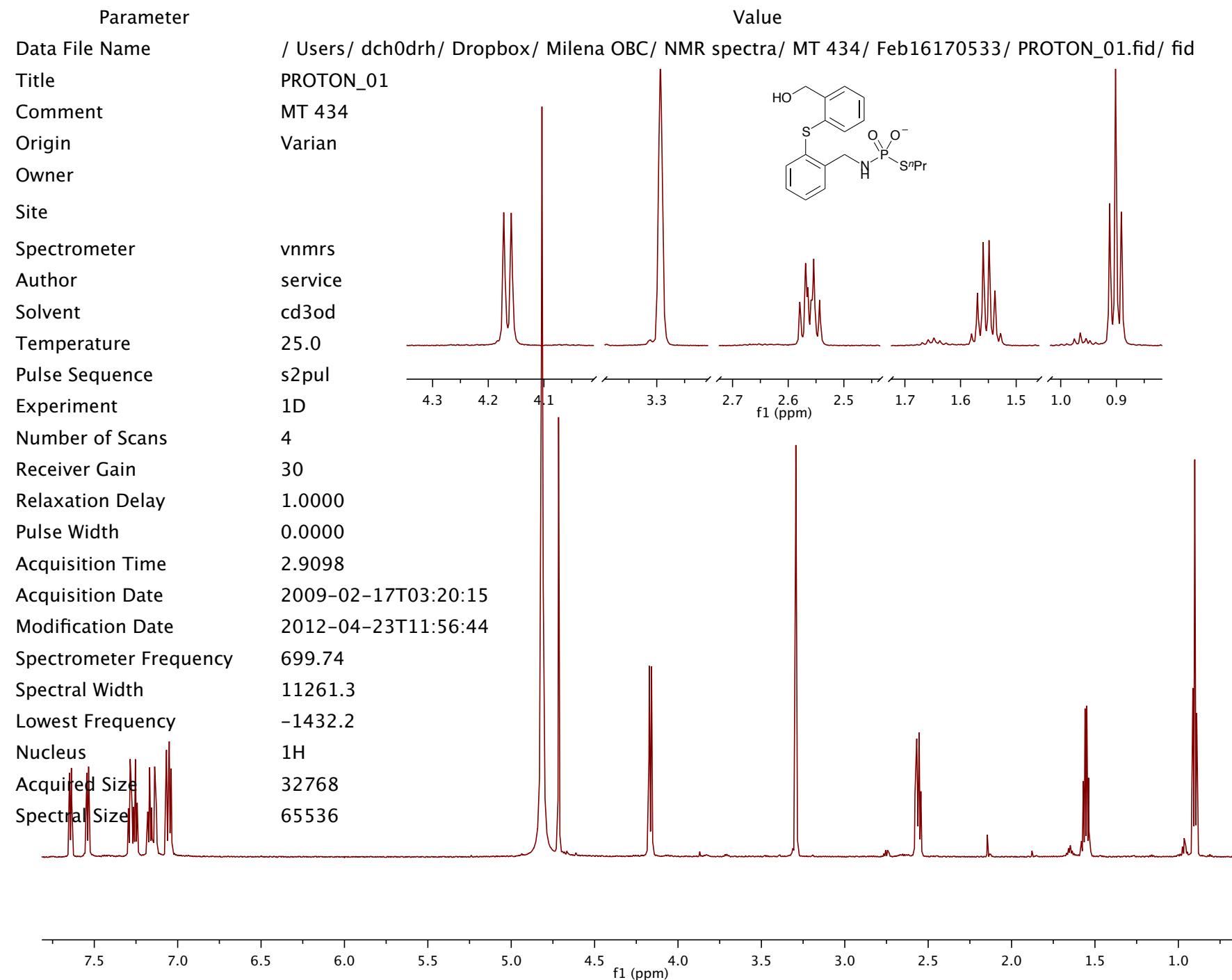
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Origin	Varian
Owner	
Site	
Spectrometer	vnmrs
Author	service
Solvent	cd3od
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	4
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	2.9098
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Modification Date	2012-04-23T11:56:54
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Acquired Size	32768
Spectral Size	65536



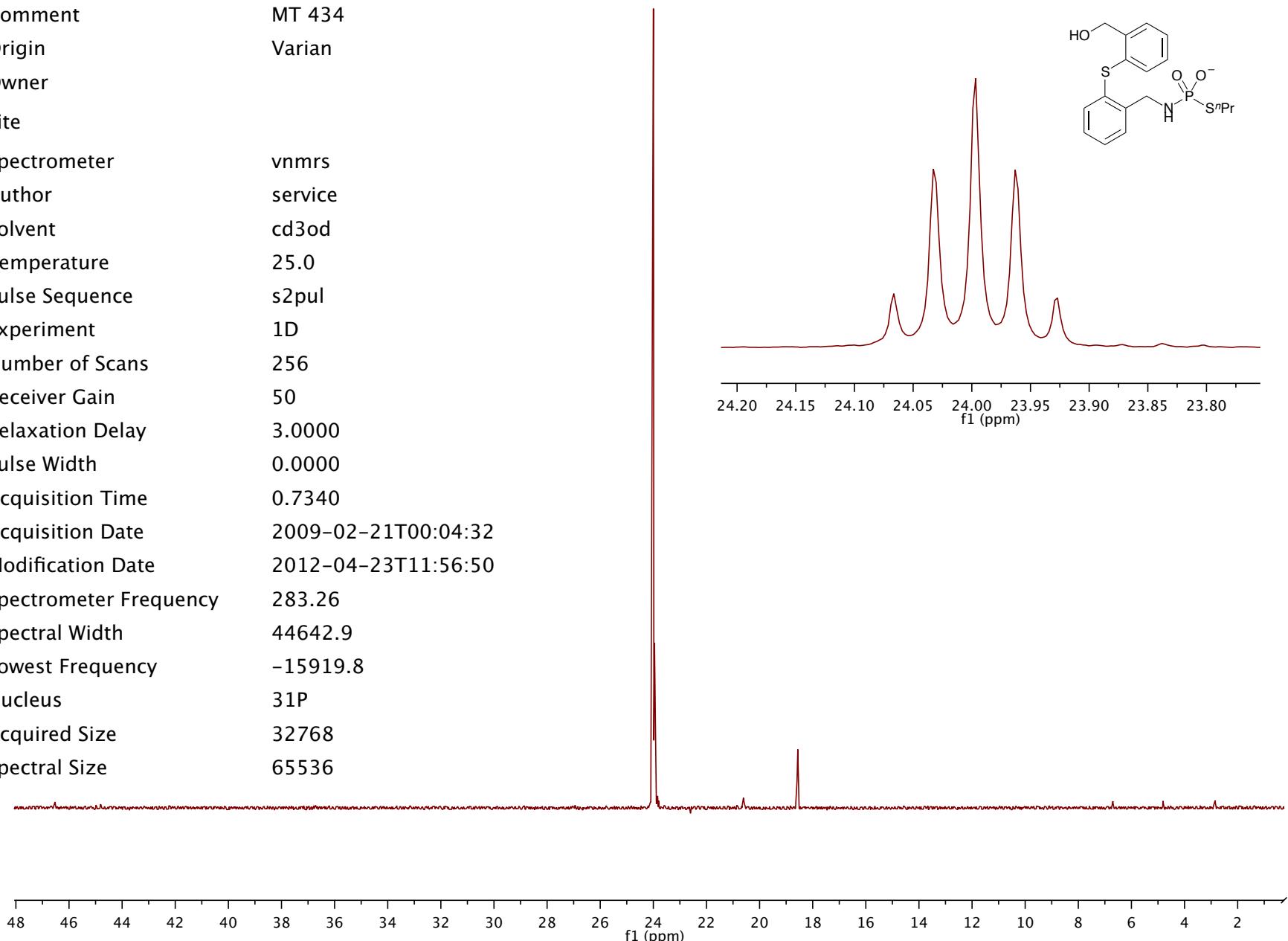
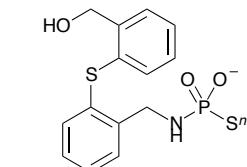
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Owner	
Site	
Spectrometer	vnmrs
Author	service
Solvent	cd3od
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	256
Receiver Gain	50
Relaxation Delay	3.0000
Pulse Width	0.0000
Acquisition Time	0.7340
Acquisition Date	2009-02-20T22:07:14
Modification Date	2012-04-23T11:56:48
Spectrometer Frequency	283.26
Spectral Width	44642.9
Lowest Frequency	-15919.8
Nucleus	³¹ P
Acquired Size	32768
Spectral Size	65536

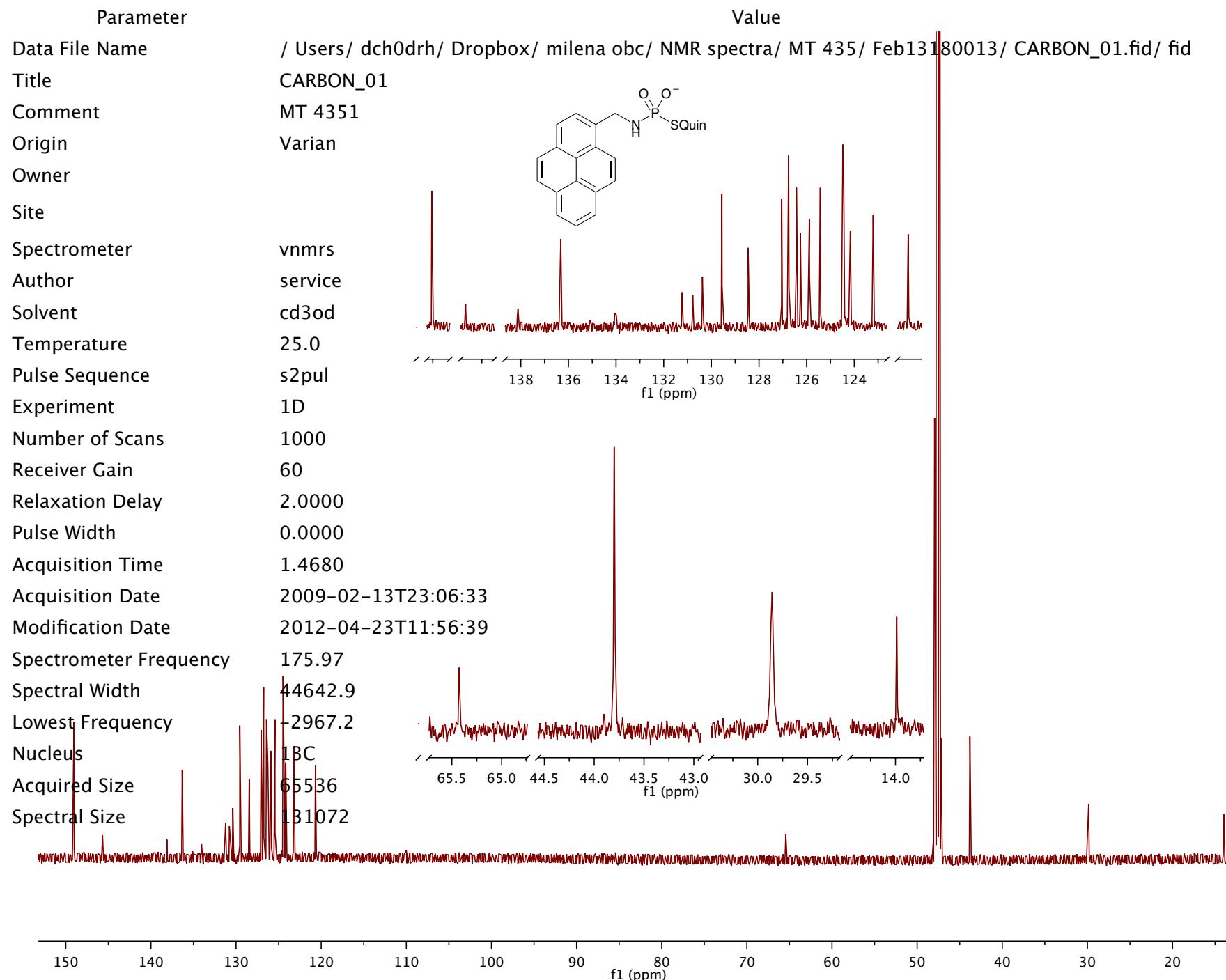


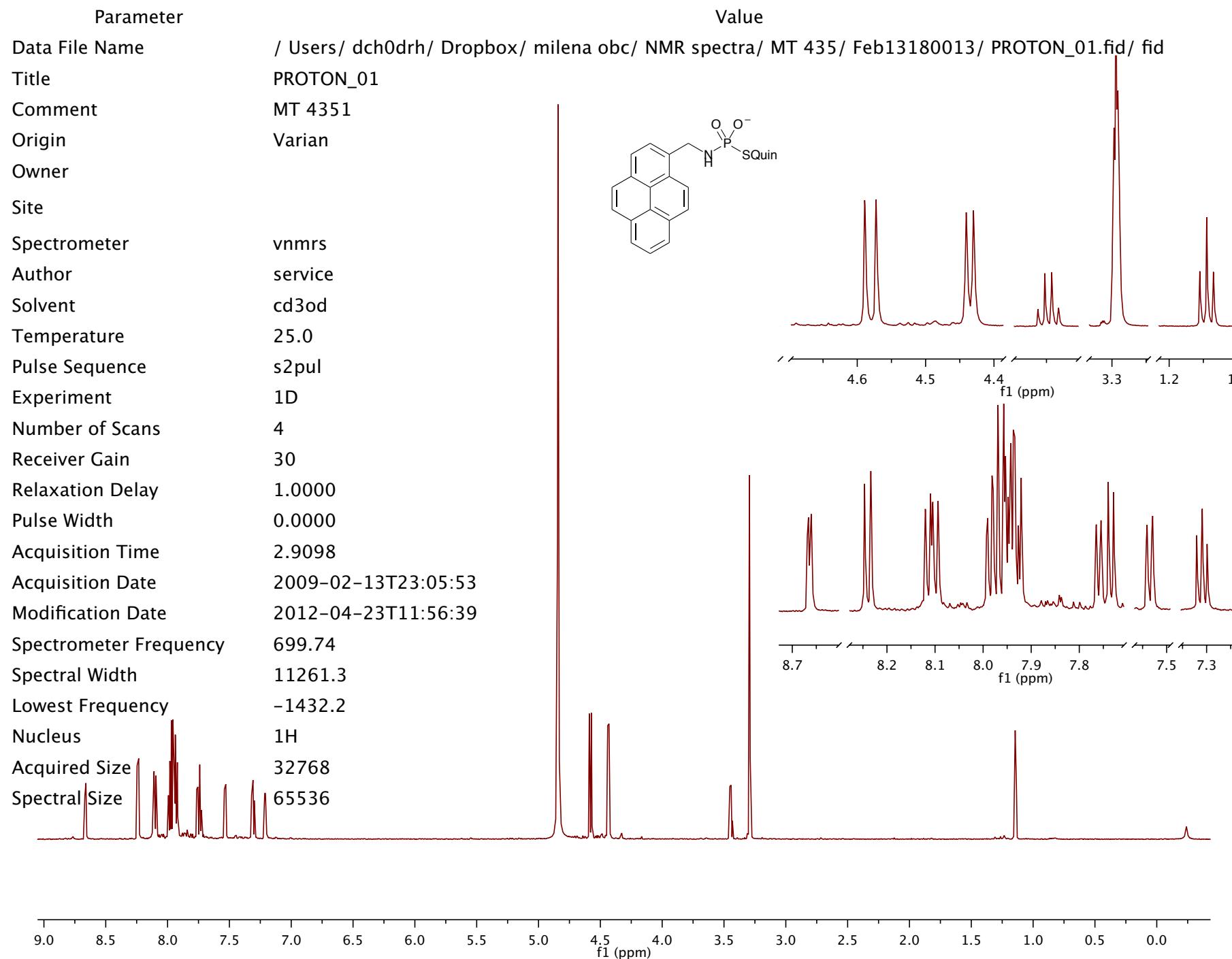




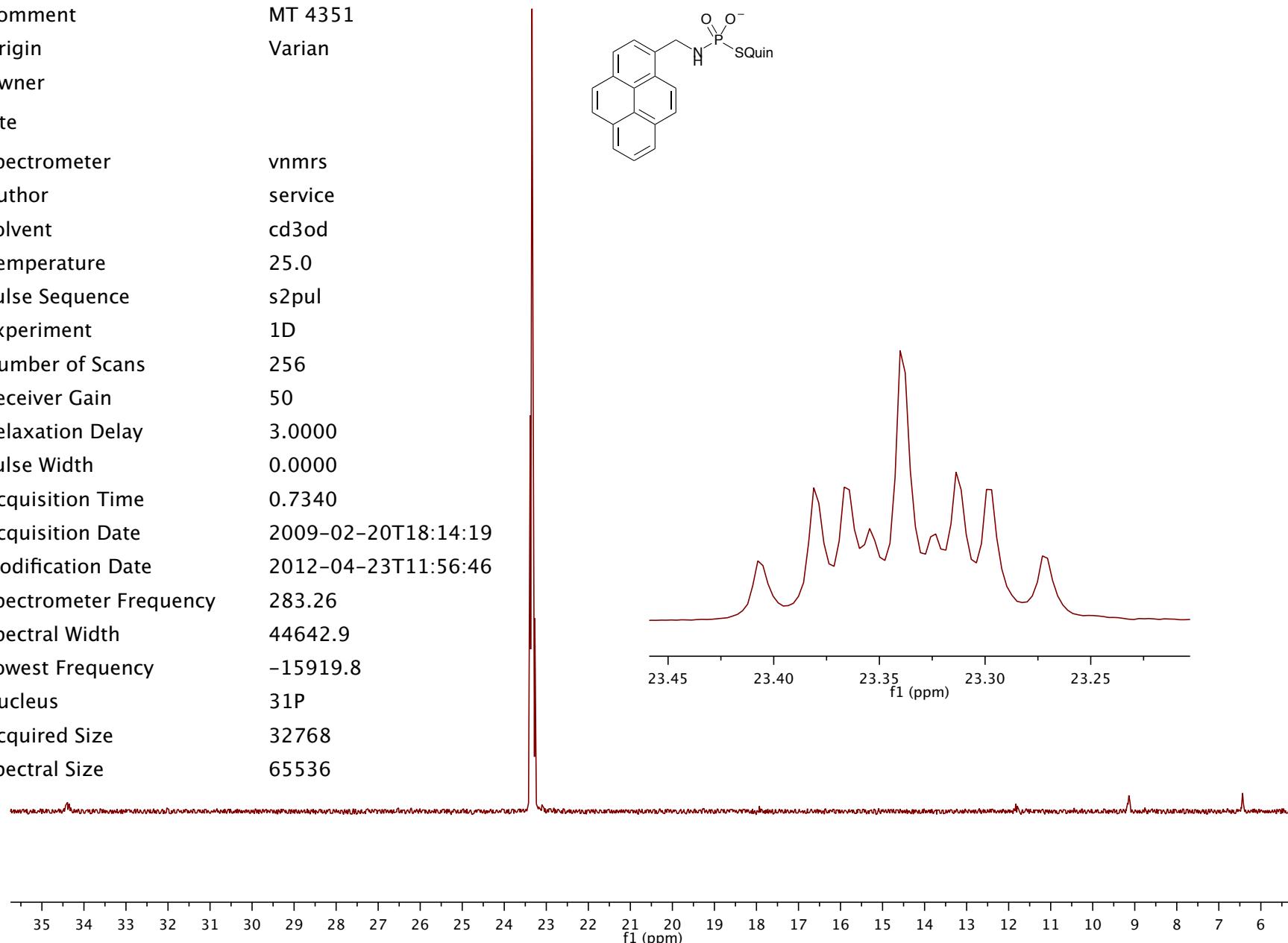
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Spectrometer	vnmrs
Author	service
Solvent	cd3od
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	256
Receiver Gain	50
Relaxation Delay	3.0000
Pulse Width	0.0000
Acquisition Time	0.7340
Acquisition Date	2009-02-21T00:04:32
Modification Date	2012-04-23T11:56:50
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Spectral Width	44642.9
Lowest Frequency	-15919.8
Nucleus	³¹ P
Acquired Size	32768
Spectral Size	65536

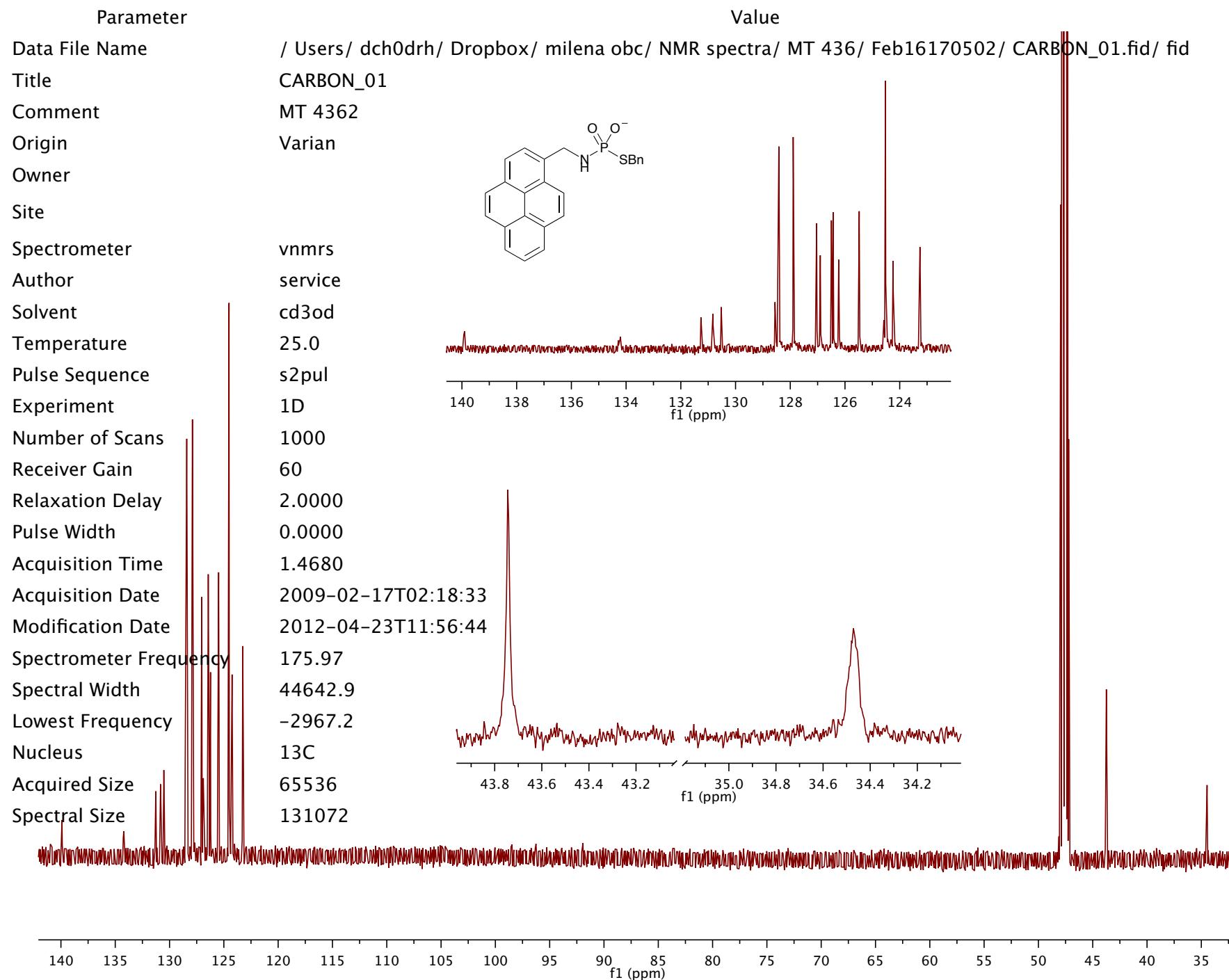


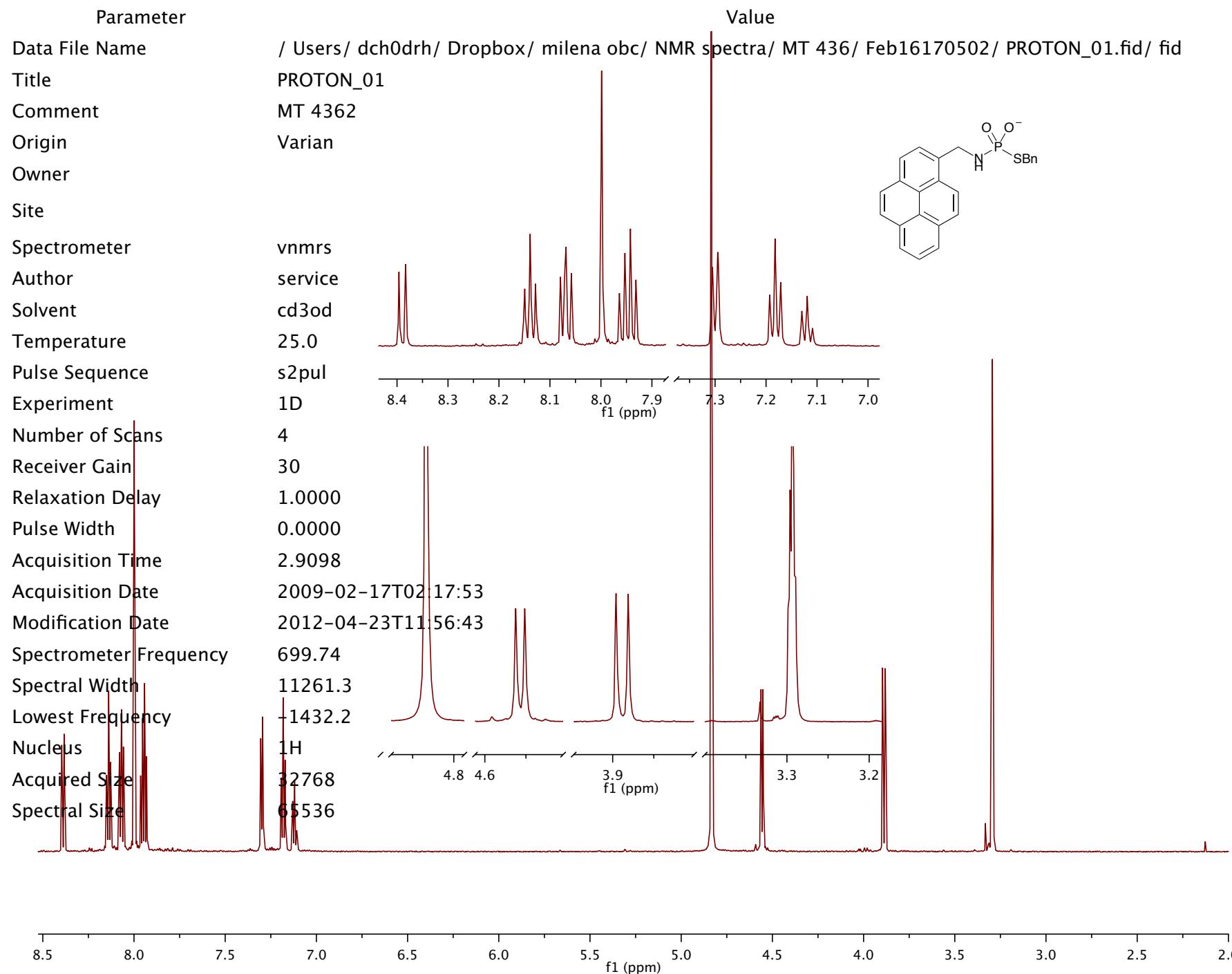




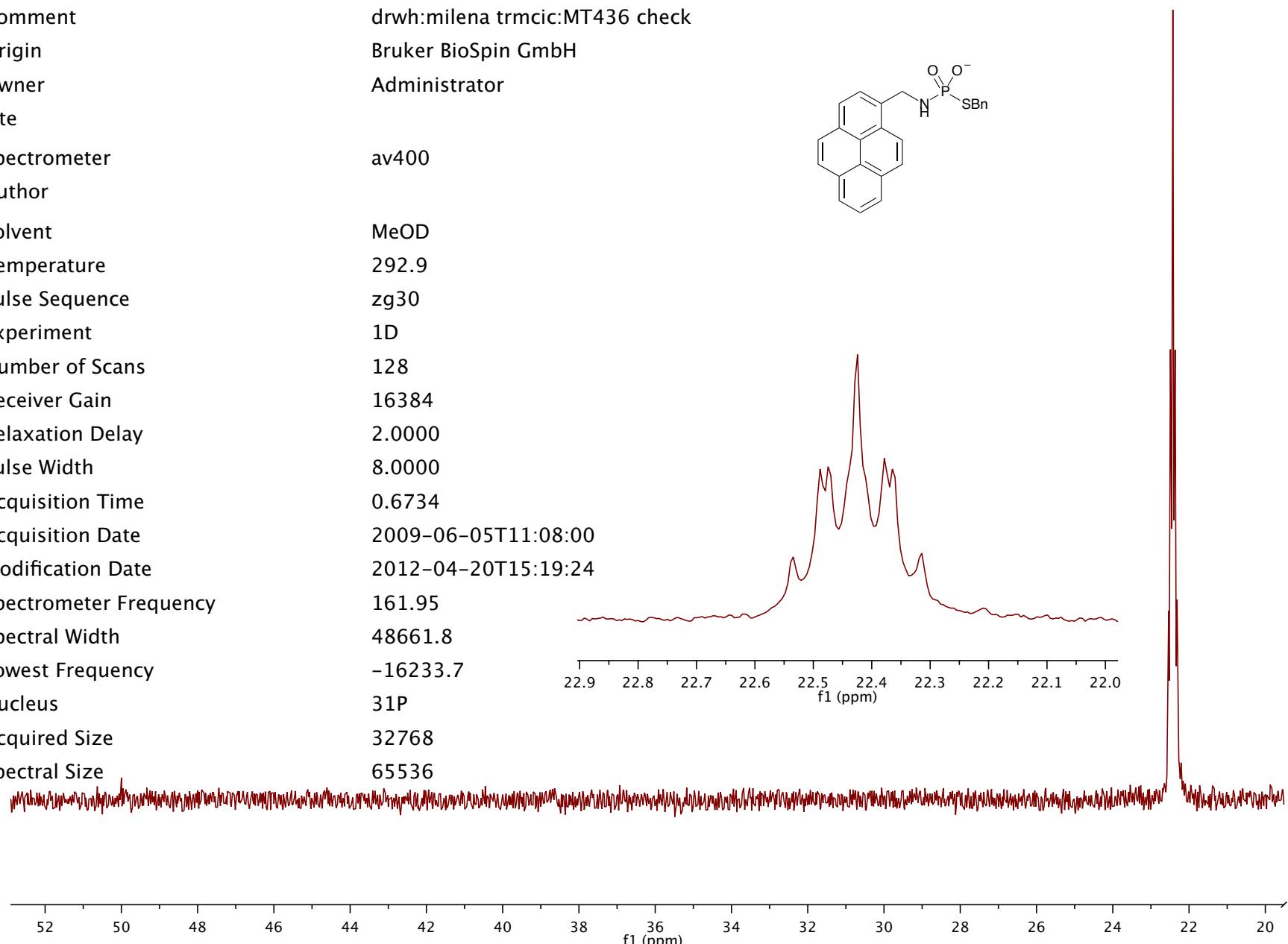
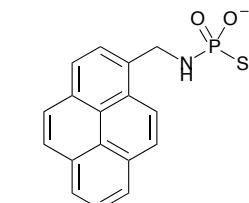
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Comment	MT 4351
Origin	Varian
Owner	
Site	
Spectrometer	vnmrs
Author	service
Solvent	cd3od
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	256
Receiver Gain	50
Relaxation Delay	3.0000
Pulse Width	0.0000
Acquisition Time	0.7340
Acquisition Date	2009-02-20T18:14:19
Modification Date	2012-04-23T11:56:46
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Spectral Width	44642.9
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Nucleus	³¹ P
Acquired Size	32768
Spectral Size	65536

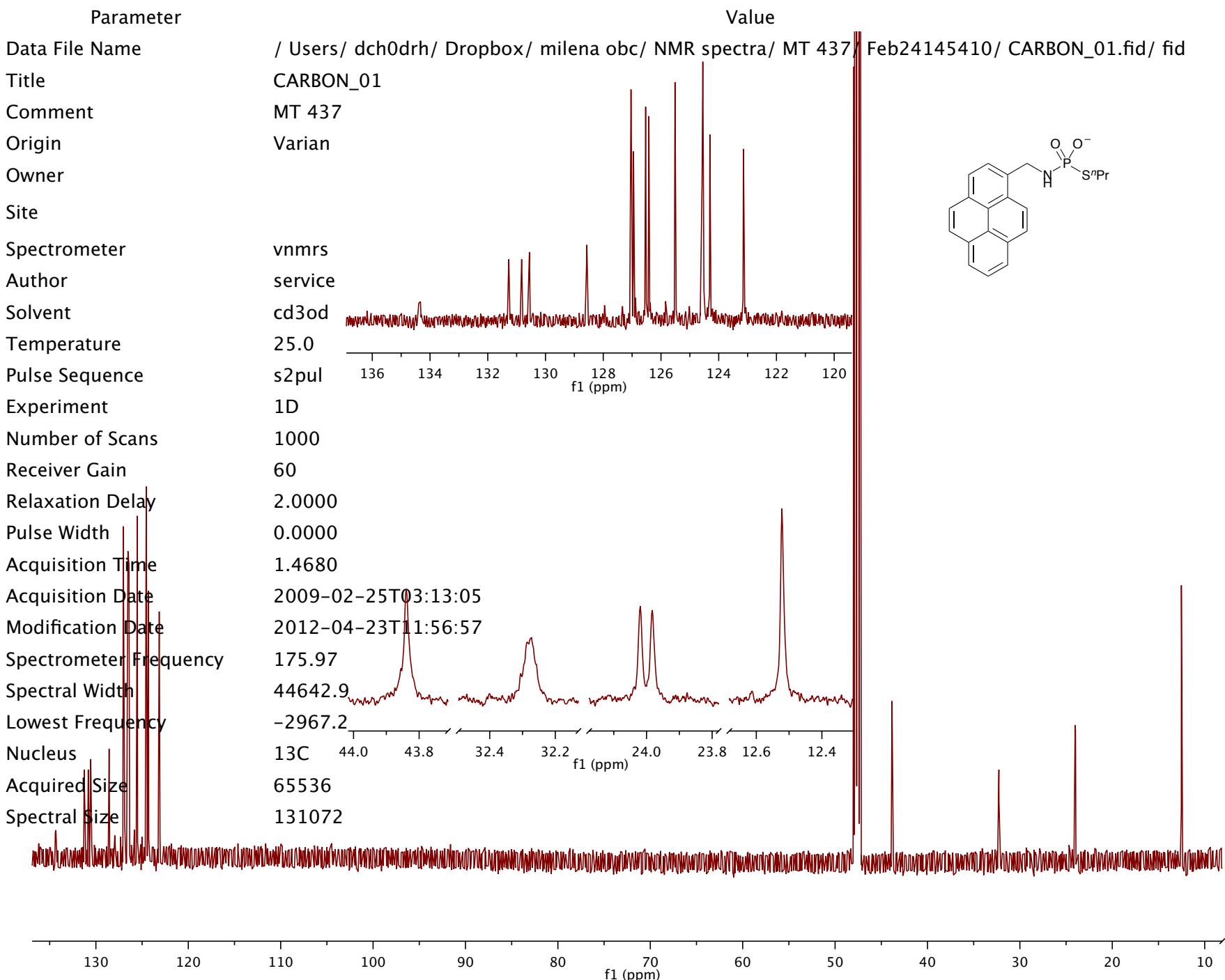


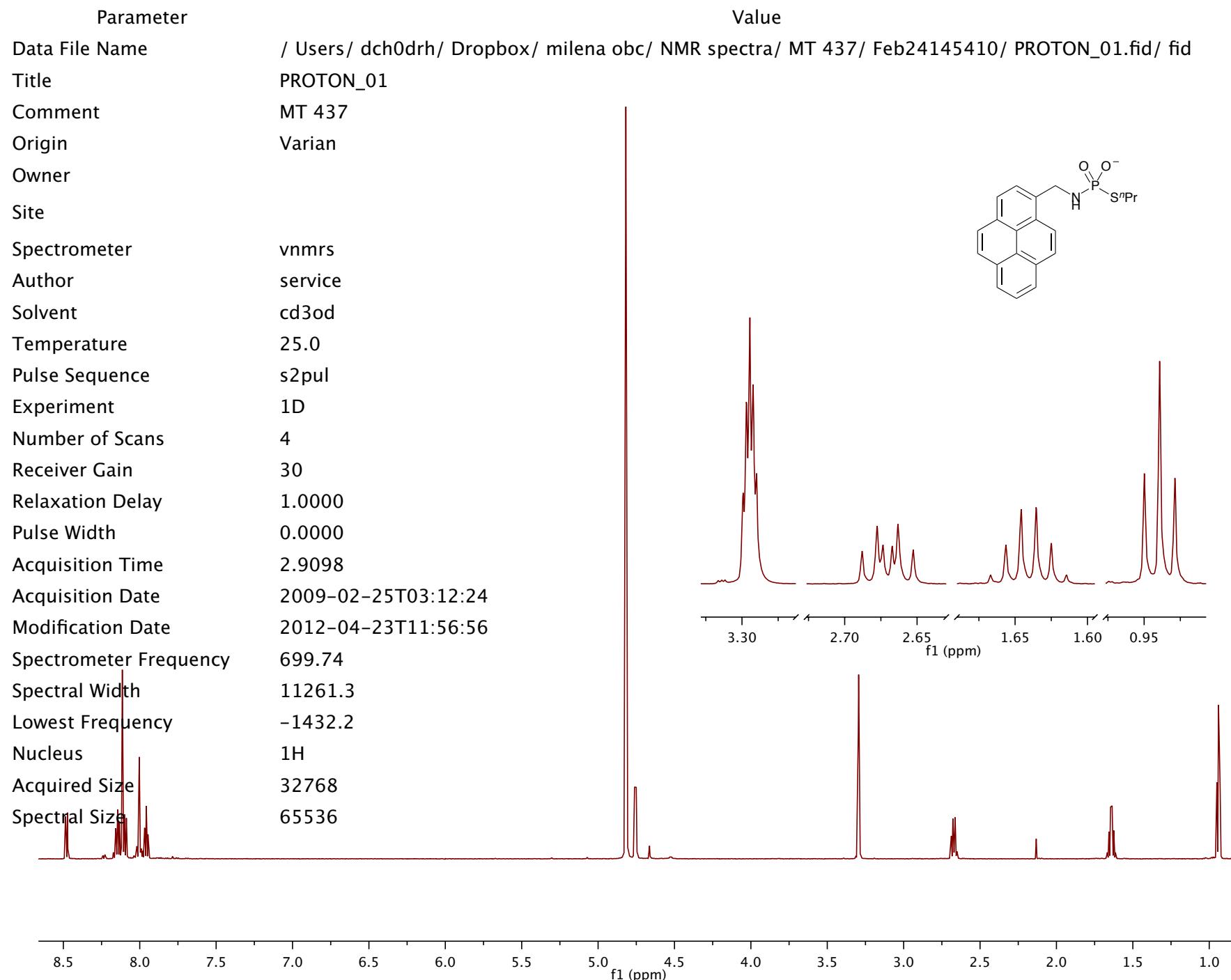




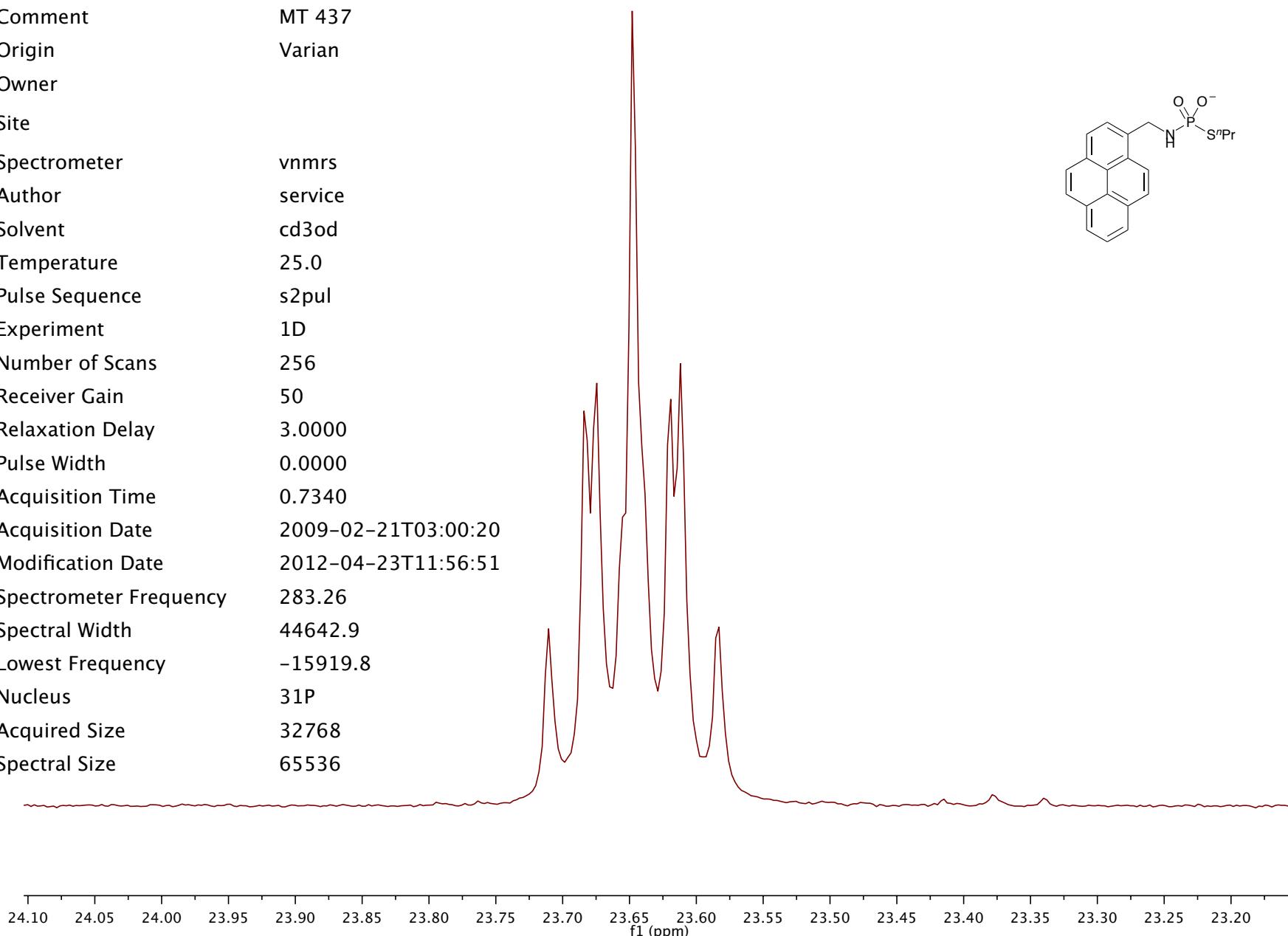
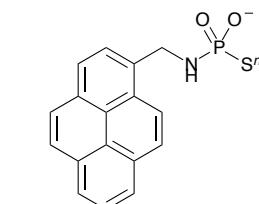
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Owner	Administrator
Site	
Spectrometer	av400
Author	
Solvent	MeOD
Temperature	292.9
Pulse Sequence	zg30
Experiment	1D
Number of Scans	128
Receiver Gain	16384
Relaxation Delay	2.0000
Pulse Width	8.0000
Acquisition Time	0.6734
Acquisition Date	2009-06-05T11:08:00
Modification Date	2012-04-20T15:19:24
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Lowest Frequency	-16233.7
Nucleus	³¹ P
Acquired Size	32768
Spectral Size	65536

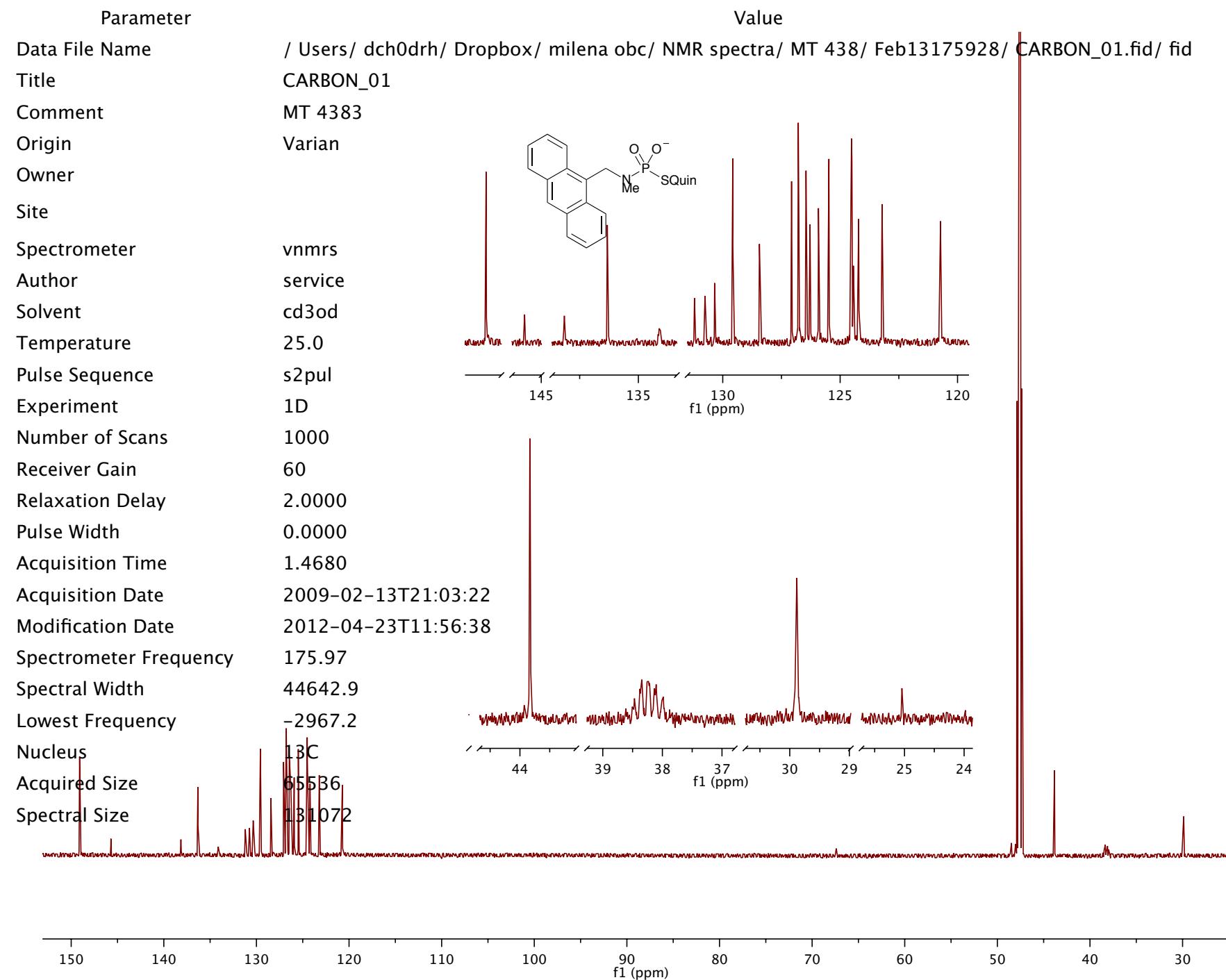


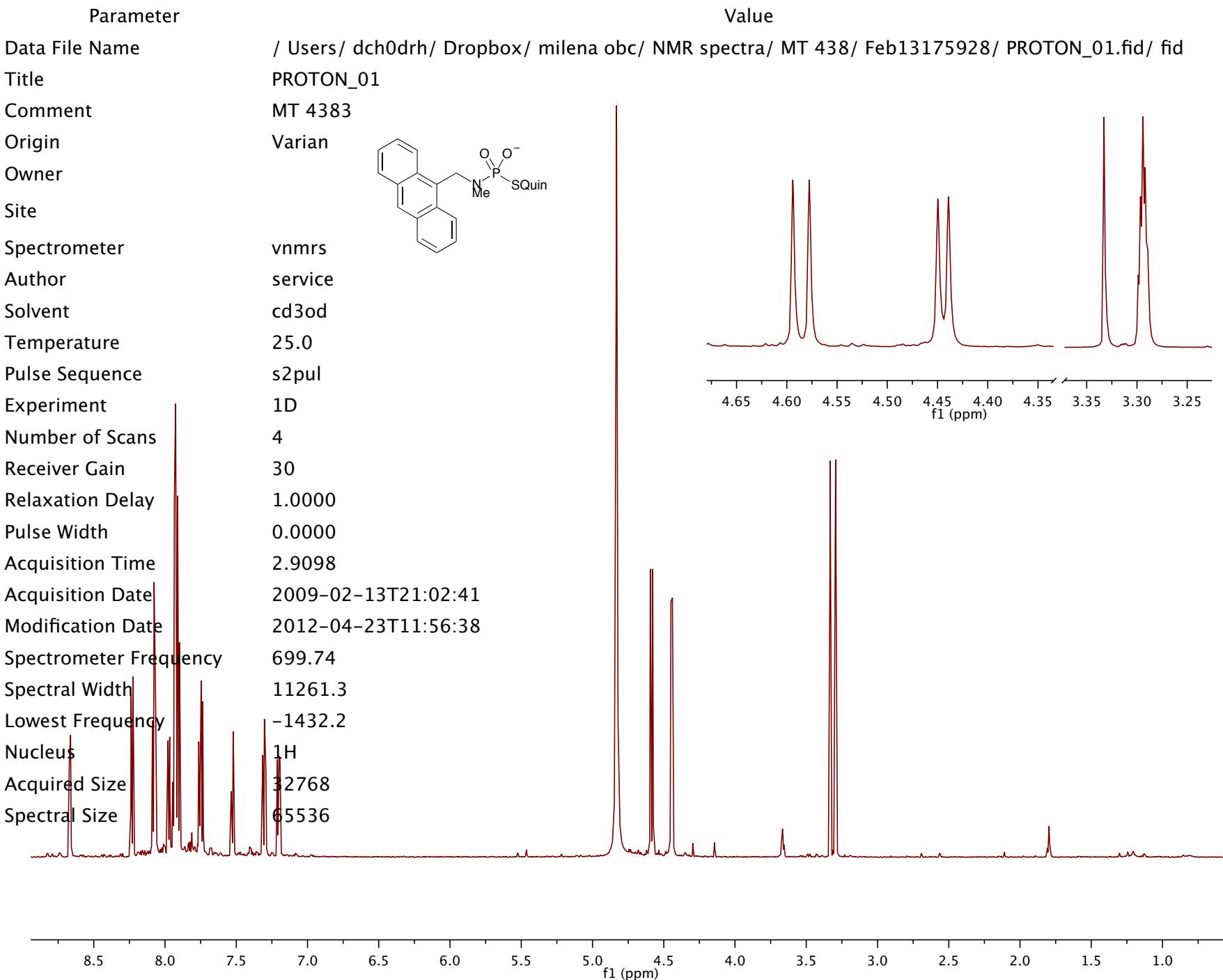




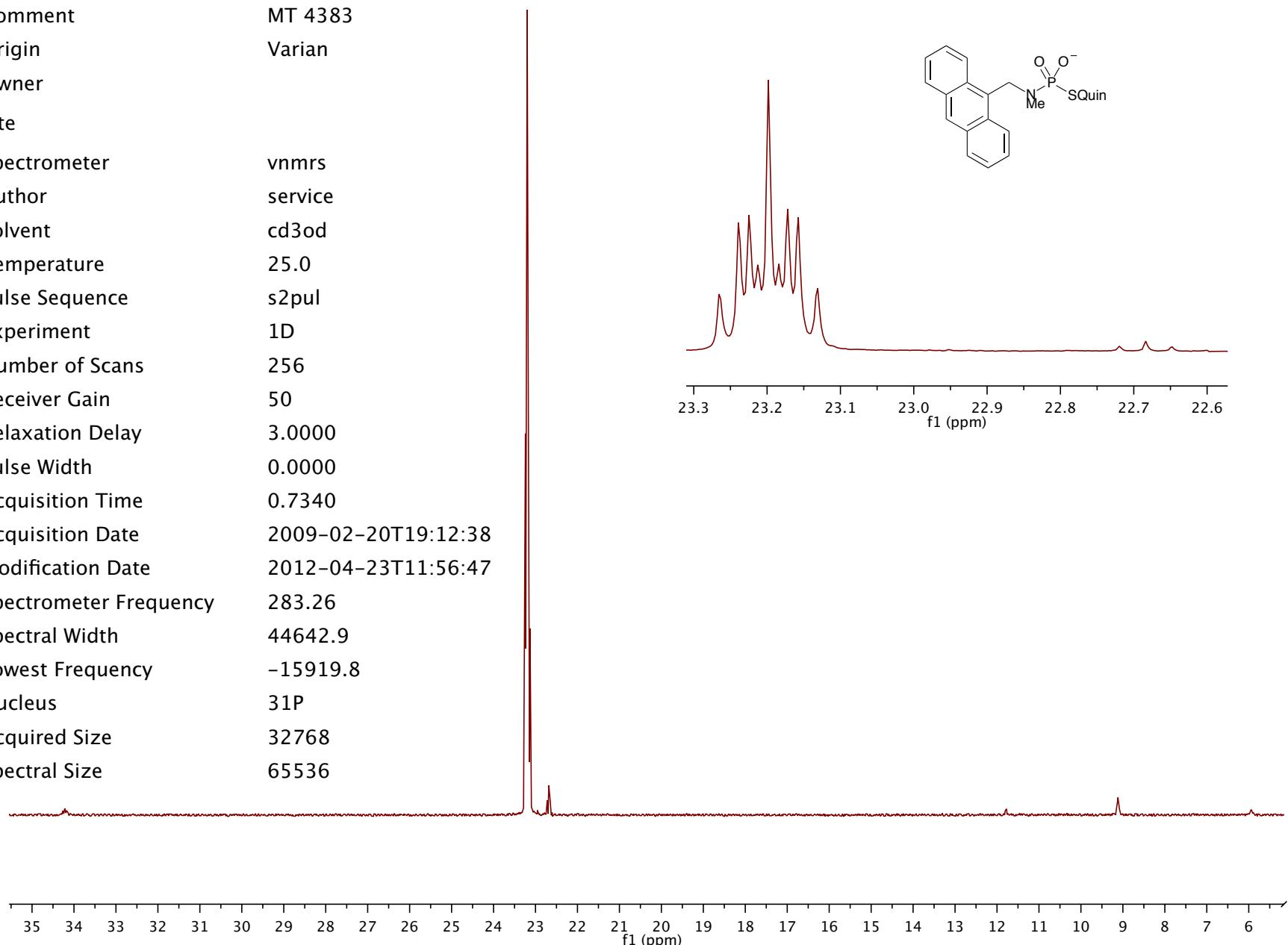
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Site	
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Author	service
Solvent	cd3od
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	256
Receiver Gain	50
Relaxation Delay	3.0000
Pulse Width	0.0000
Acquisition Time	0.7340
Acquisition Date	2009-02-21T03:00:20
Modification Date	2012-04-23T11:56:51
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Spectral Width	44642.9
Lowest Frequency	-15919.8
Nucleus	³¹ P
Acquired Size	32768
Spectral Size	65536

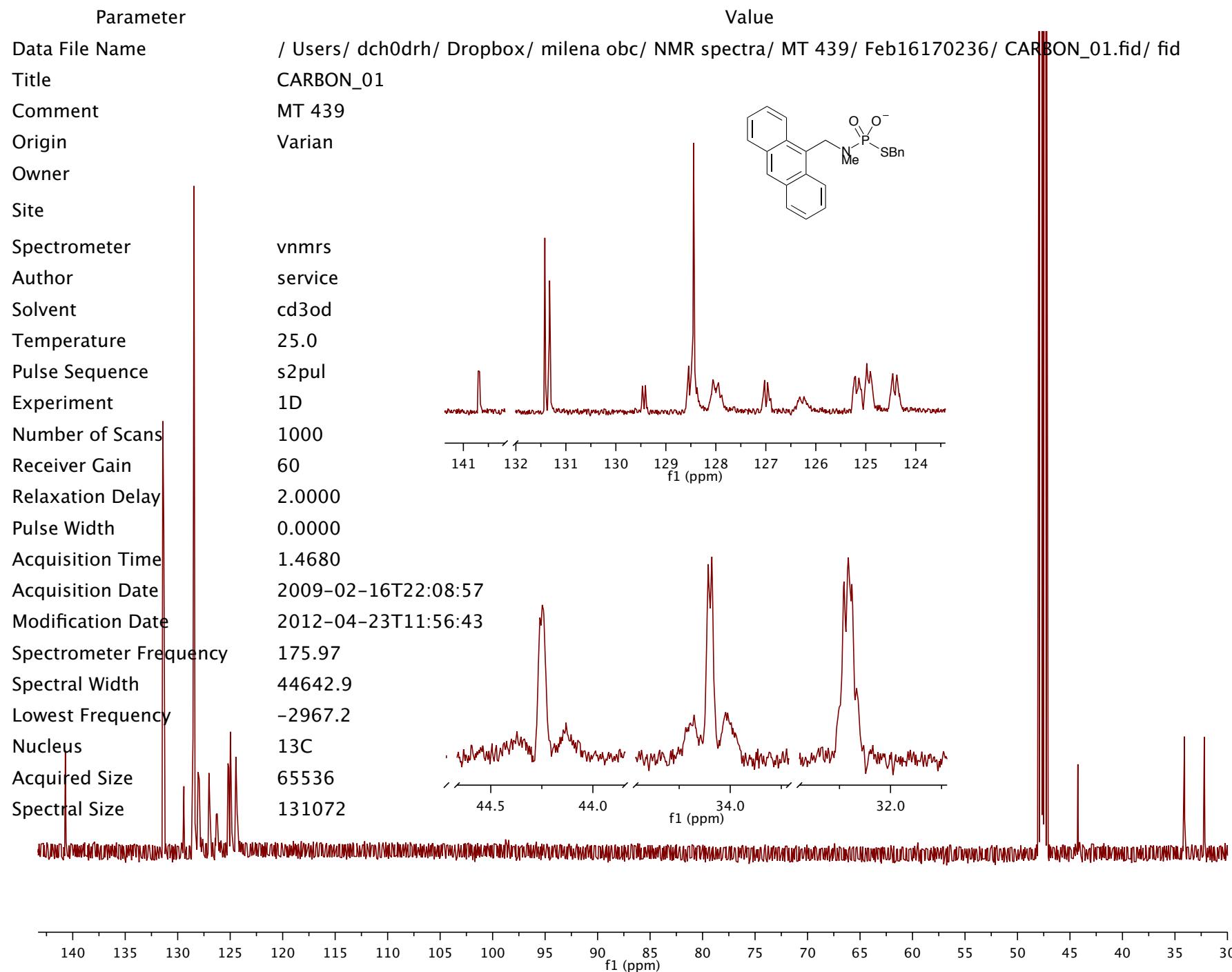


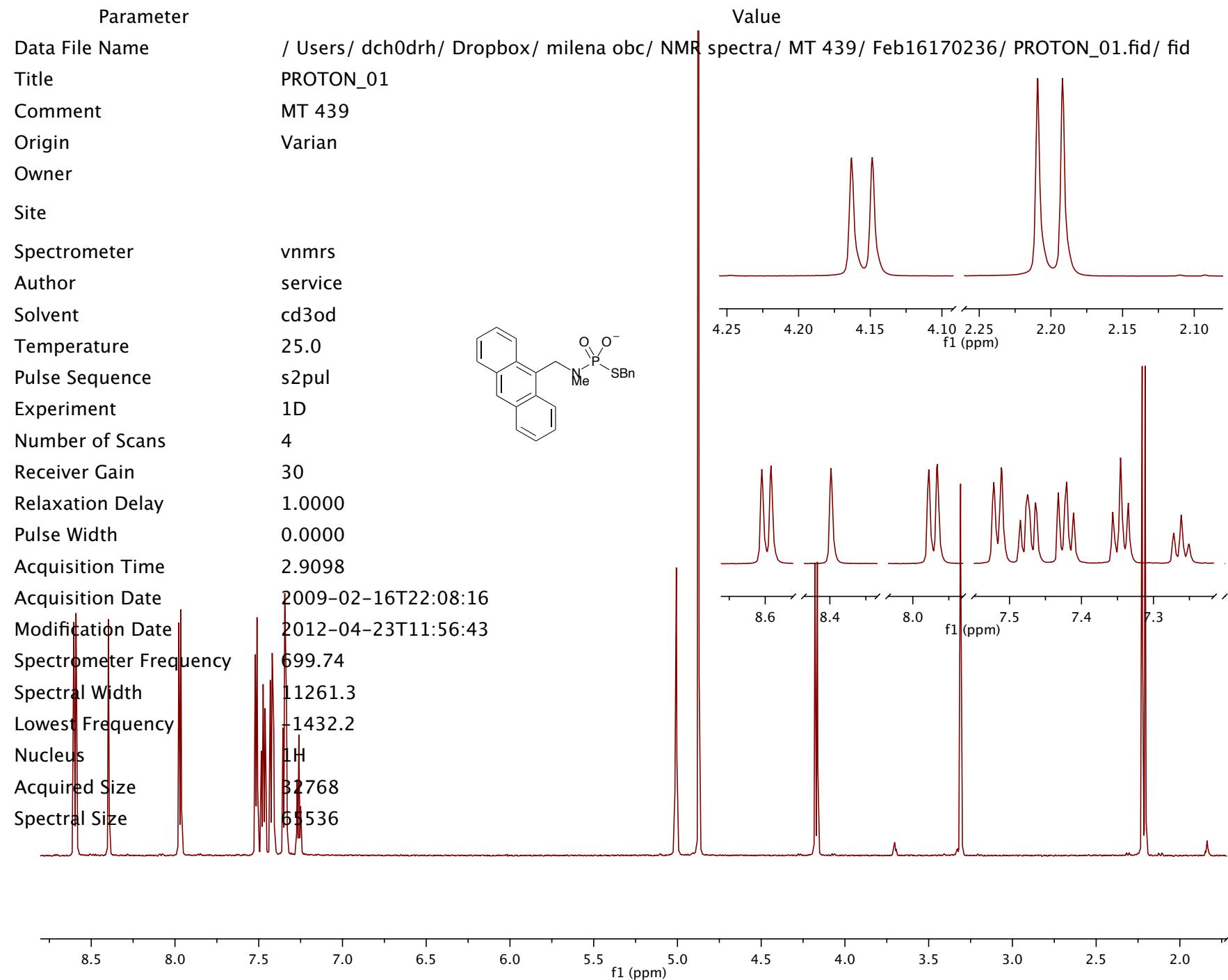




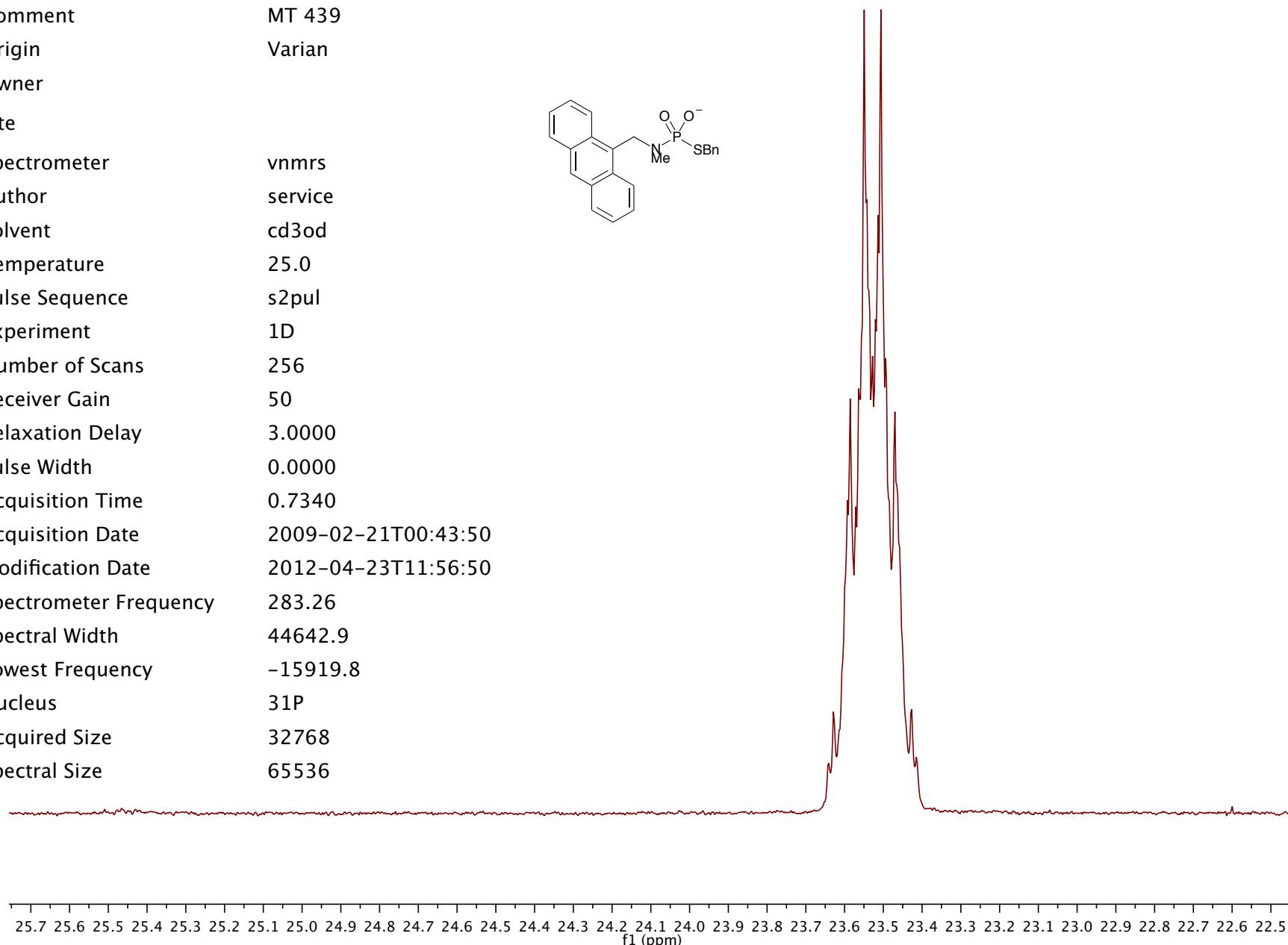
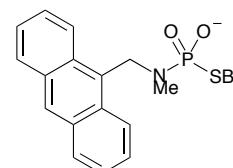
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Site	
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Author	service
Solvent	cd3od
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	256
Receiver Gain	50
Relaxation Delay	3.0000
Pulse Width	0.0000
Acquisition Time	0.7340
Acquisition Date	2009-02-20T19:12:38
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Nucleus	³¹ P
Acquired Size	32768
Spectral Size	65536

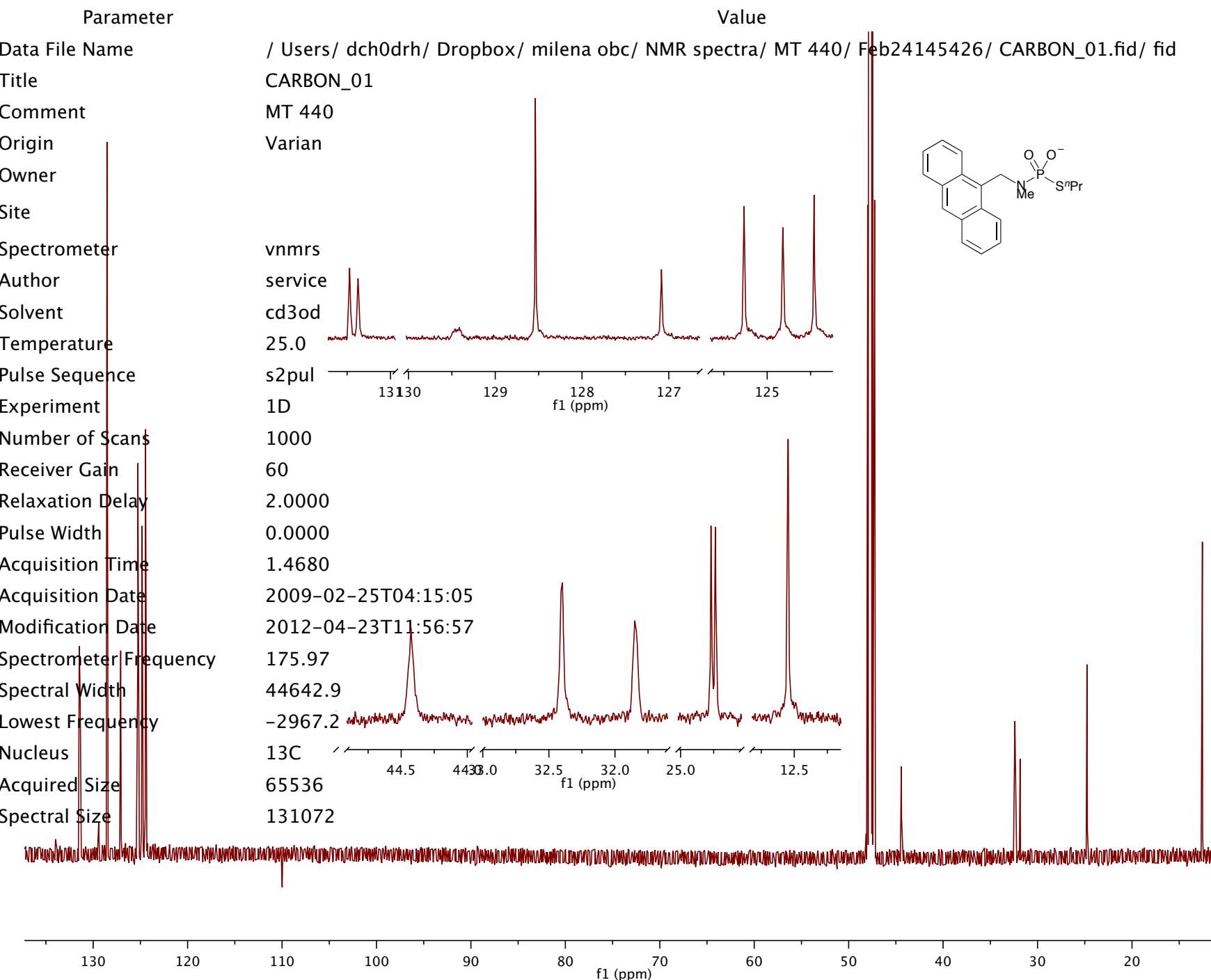


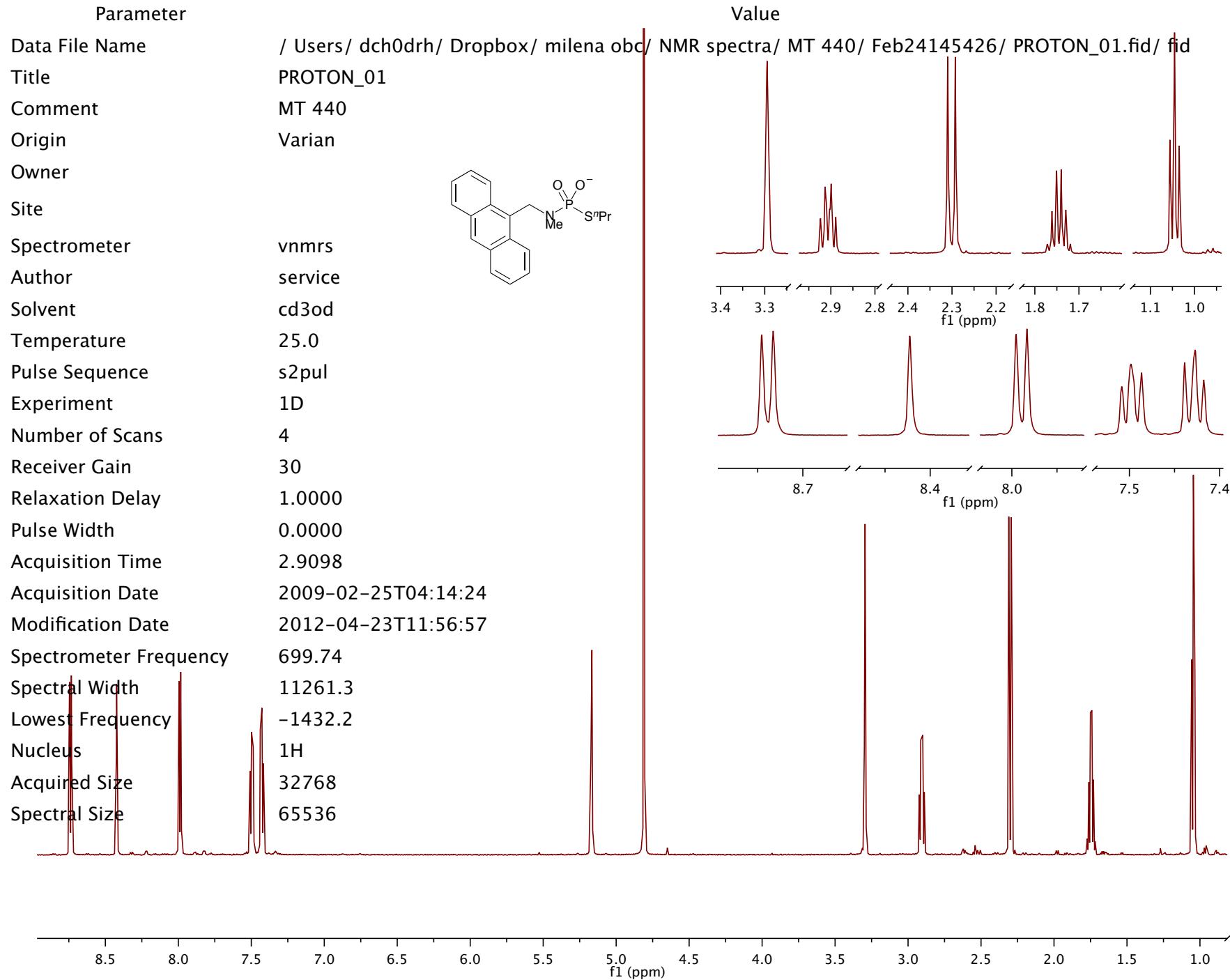


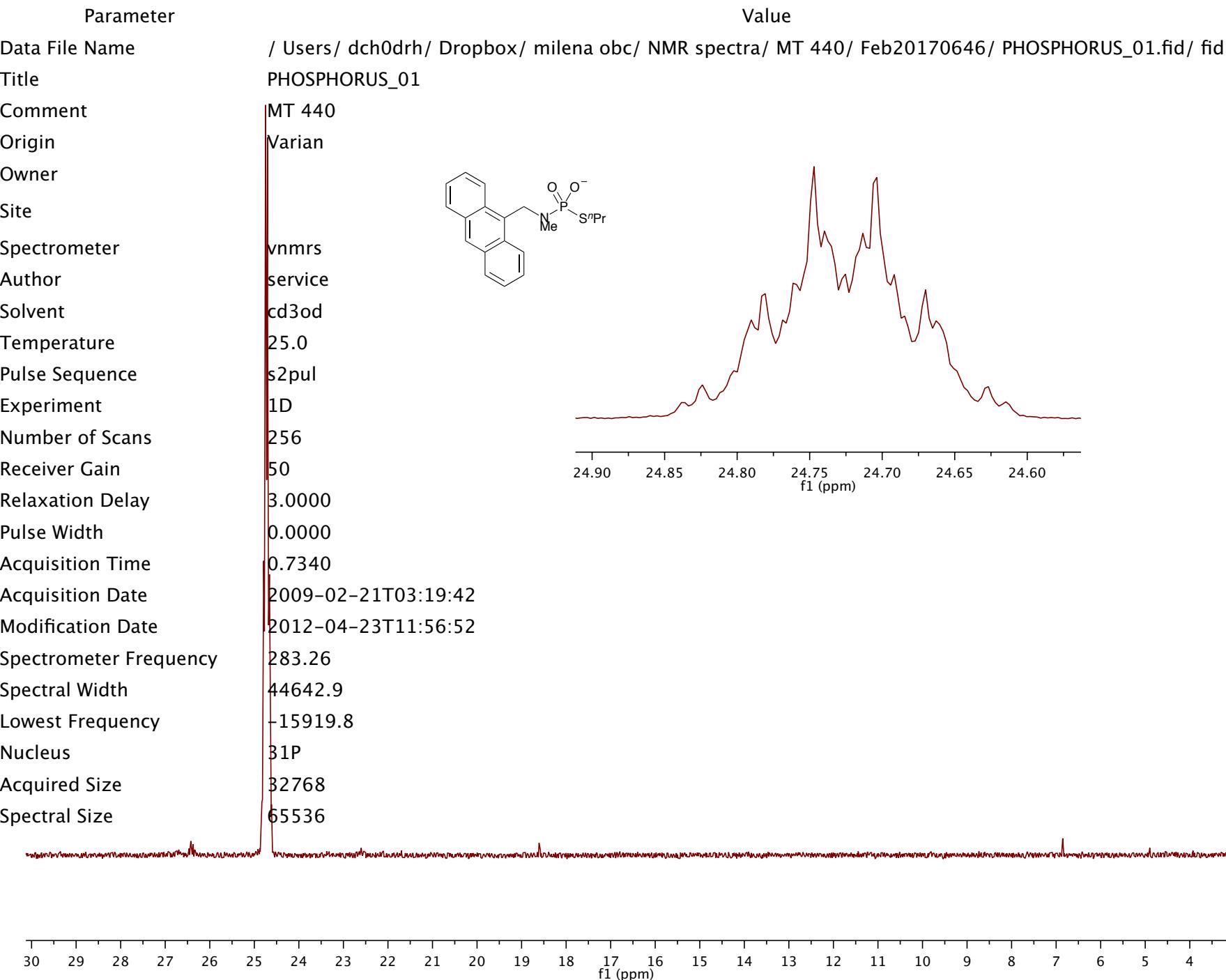


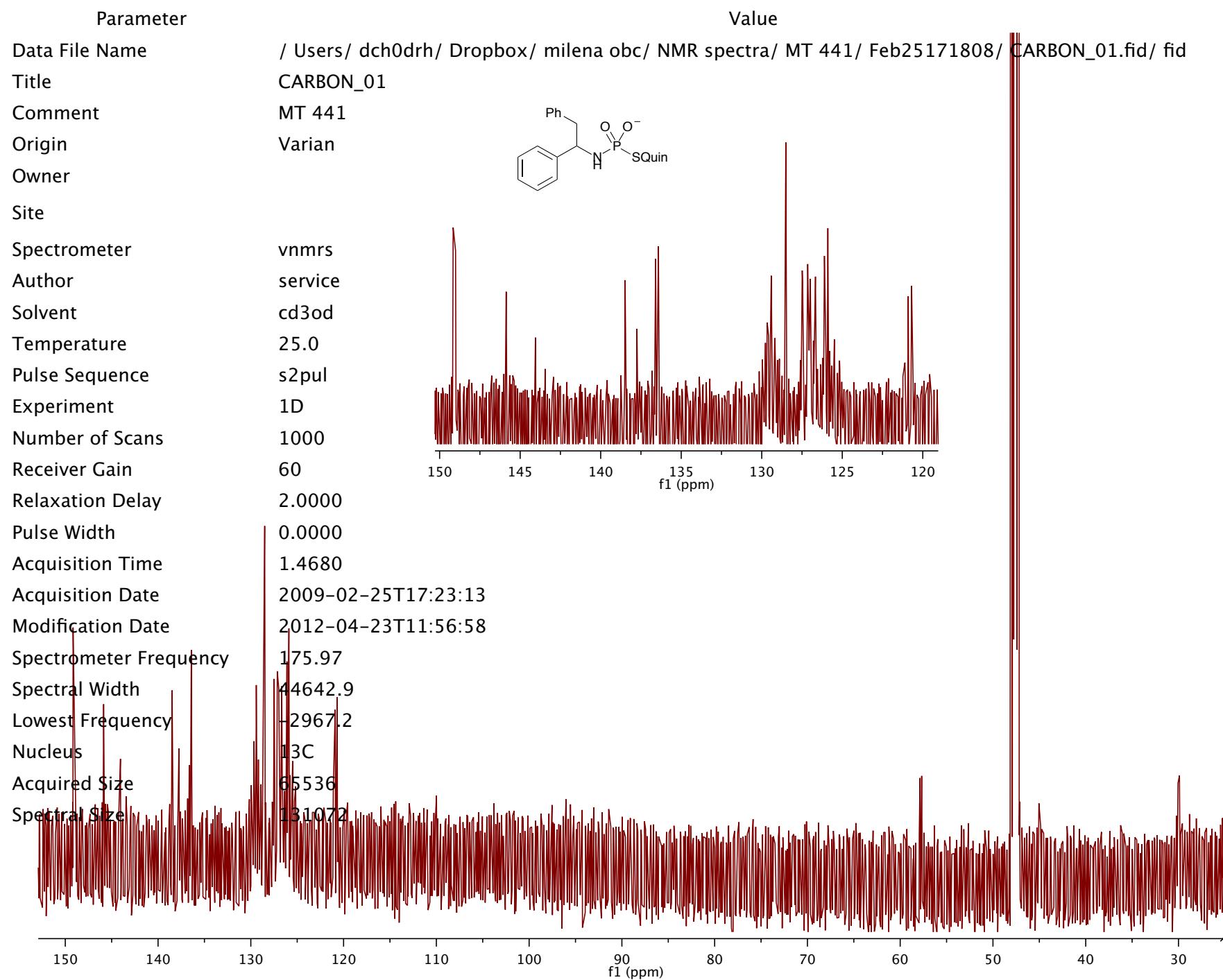
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Site	
Spectrometer	vnmrs
Author	service
Solvent	cd3od
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	256
Receiver Gain	50
Relaxation Delay	3.0000
Pulse Width	0.0000
Acquisition Time	0.7340
Acquisition Date	2009-02-21T00:43:50
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Lowest Frequency	-15919.8
Nucleus	³¹ P
Acquired Size	32768
Spectral Size	65536

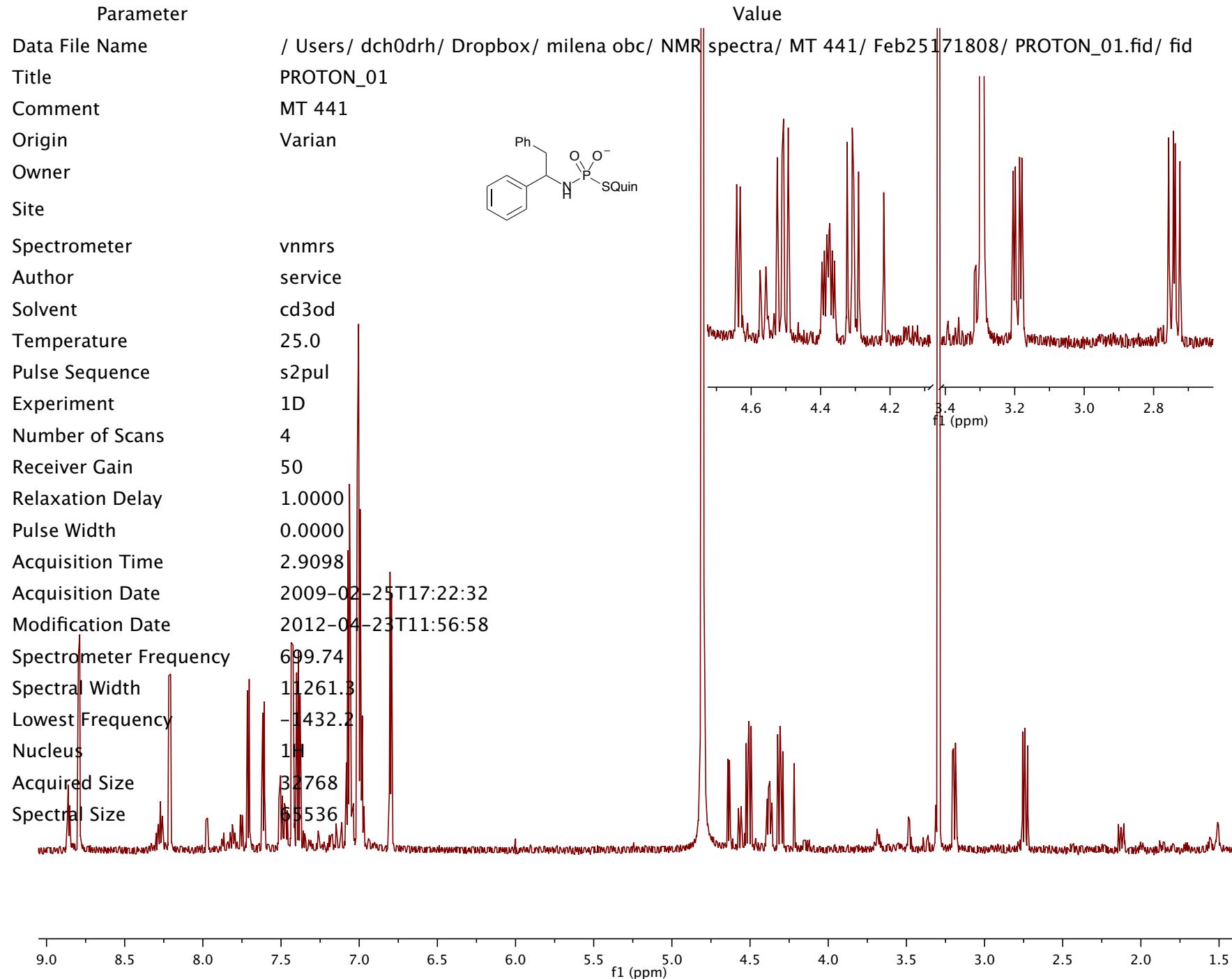


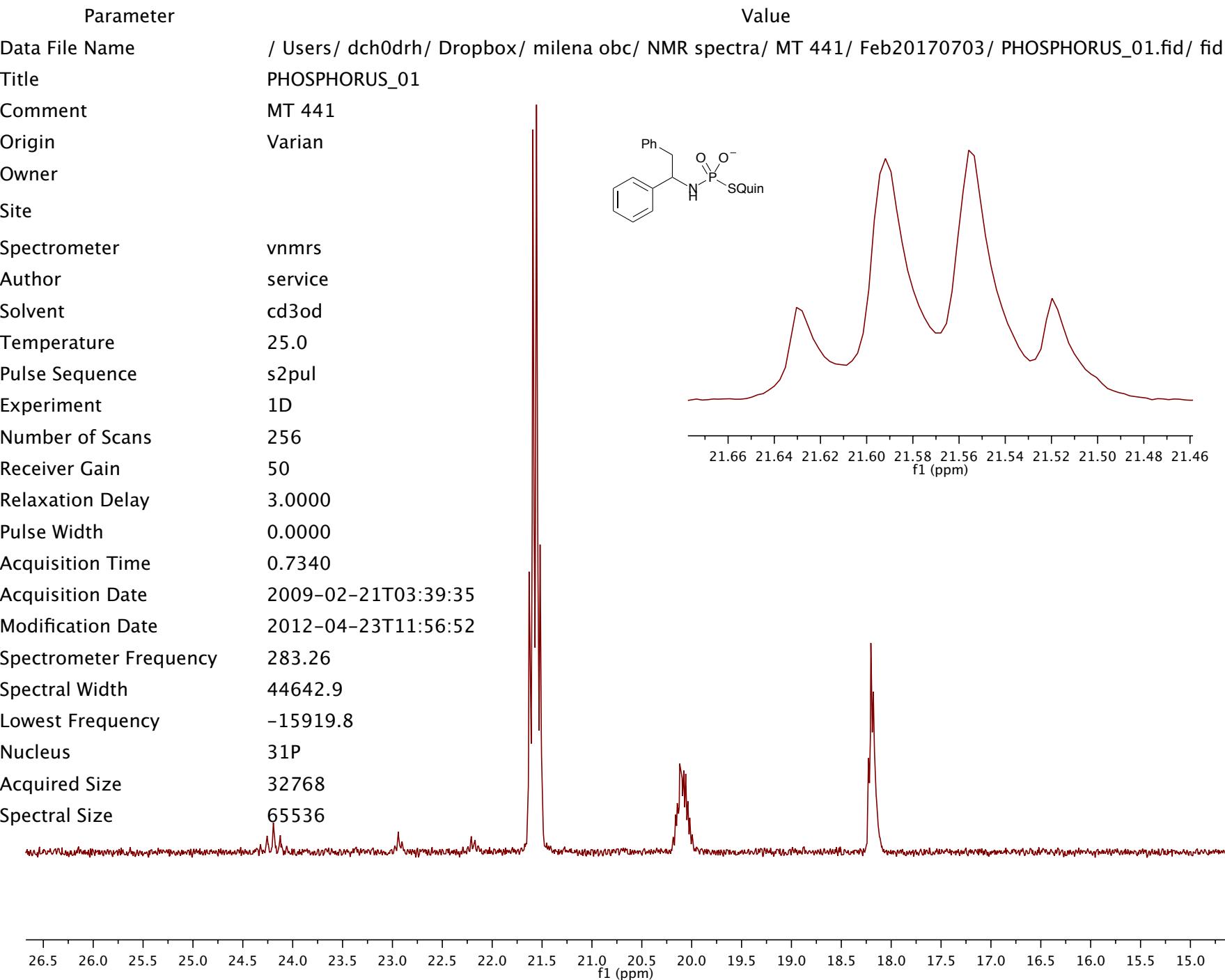








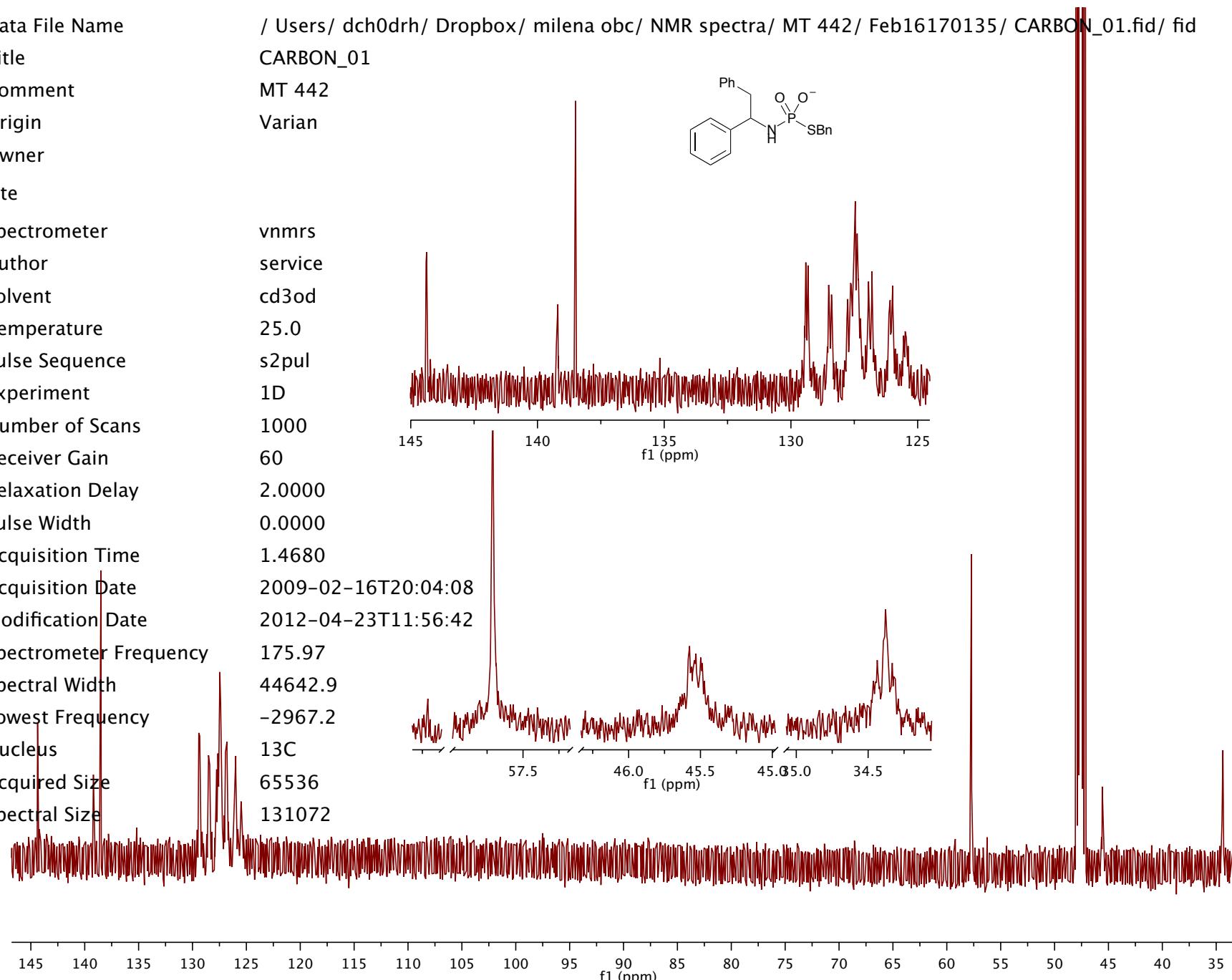
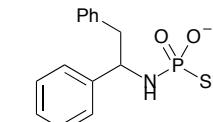


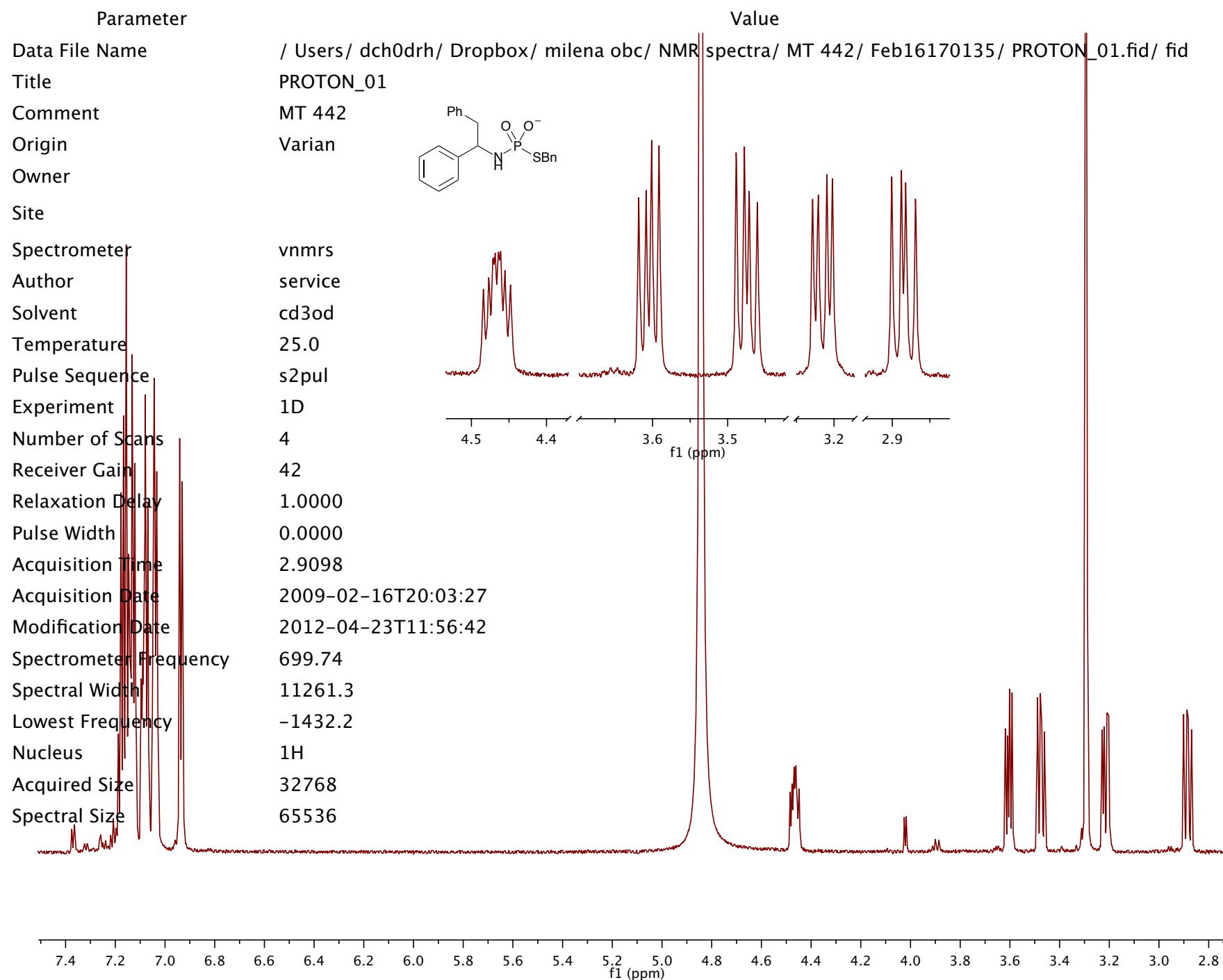


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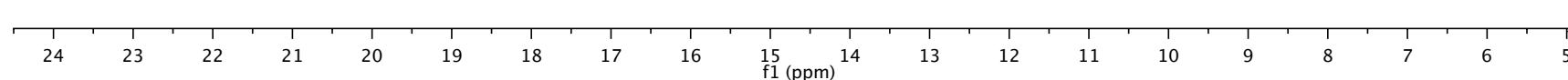
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Site	
Spectrometer	vnmrs
Author	service
Solvent	cd3od
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	1000
Receiver Gain	60
Relaxation Delay	2.0000
Pulse Width	0.0000
Acquisition Time	1.4680
Acquisition Date	2009-02-16T20:04:08
Modification Date	2012-04-23T11:56:42
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Lowest Frequency	-2967.2
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Acquired Size	65536
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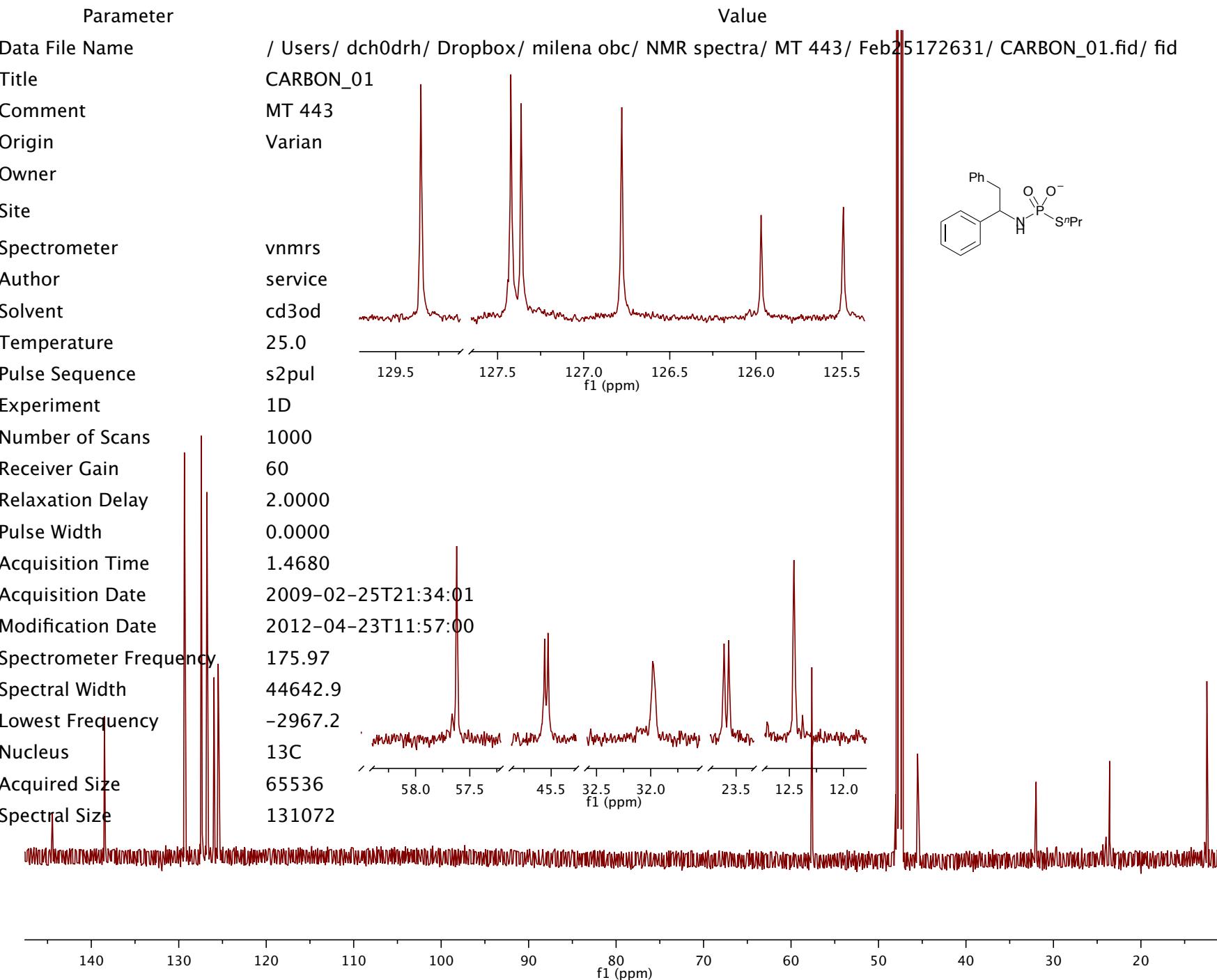
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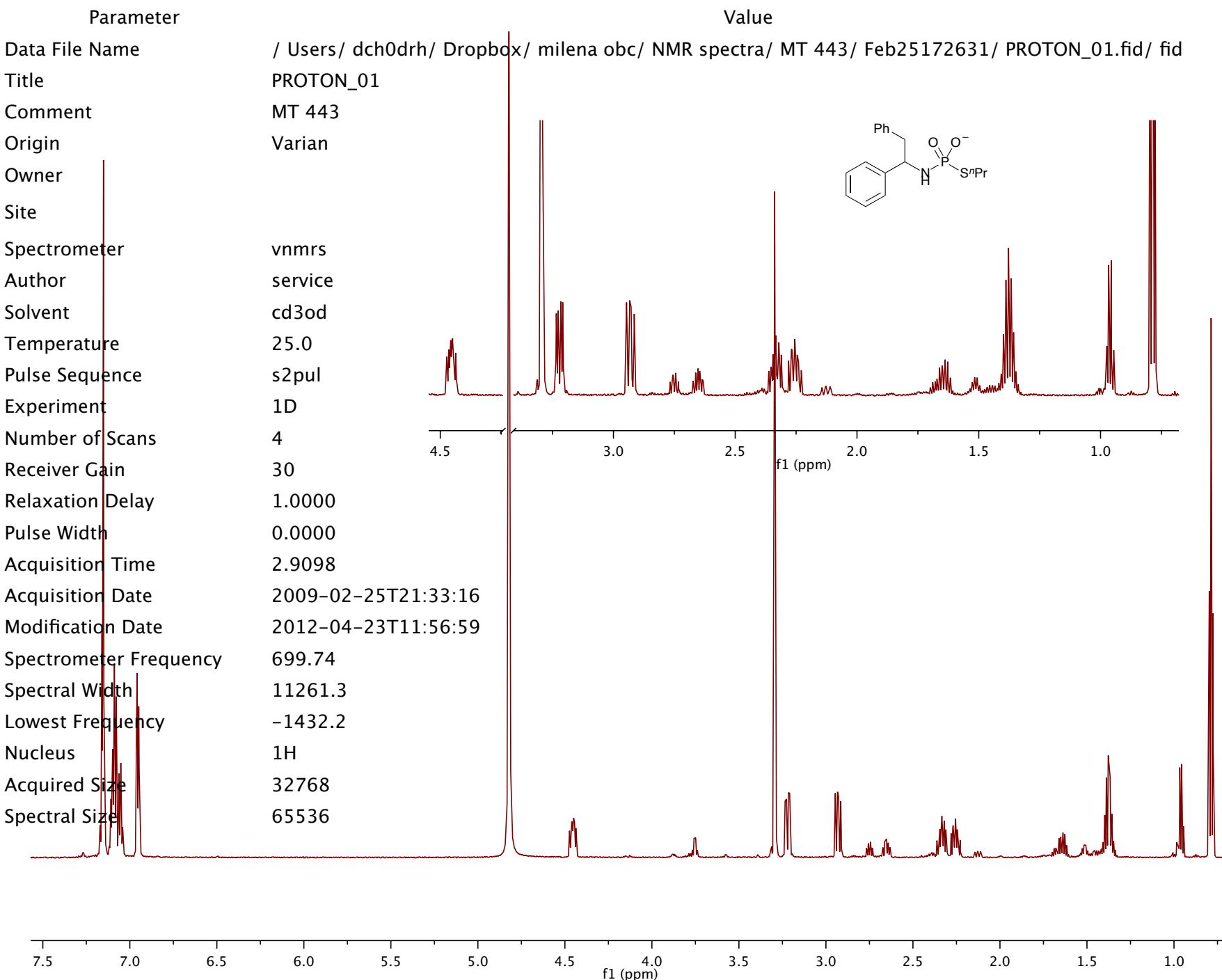




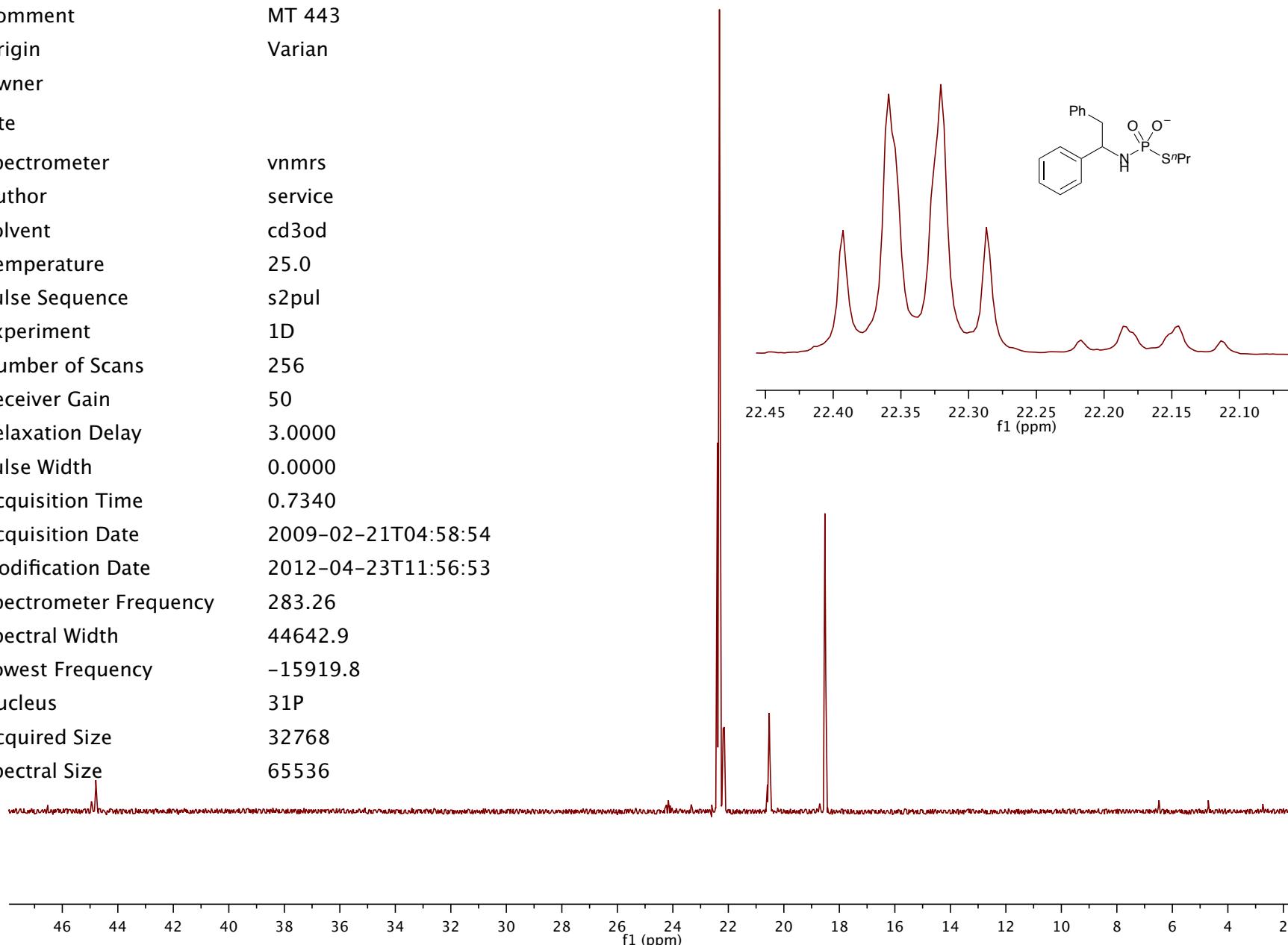
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Spectrometer	vnmrs
Author	service
Solvent	cd3od
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Pulse Sequence	s2pul
Experiment	1D
Number of Scans	256
Receiver Gain	50
Relaxation Delay	3.0000
Pulse Width	0.0000
Acquisition Time	0.7340
Acquisition Date	2009-02-21T01:03:14
Modification Date	2012-04-23T11:56:50
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Spectral Width	44642.9
Lowest Frequency	-15919.8
Nucleus	³¹ P
Acquired Size	32768
Spectral Size	65536



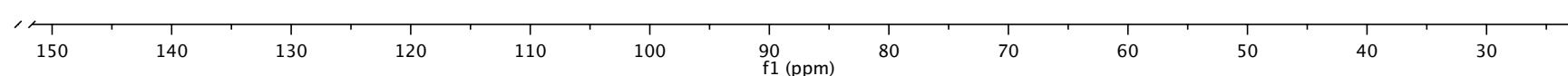




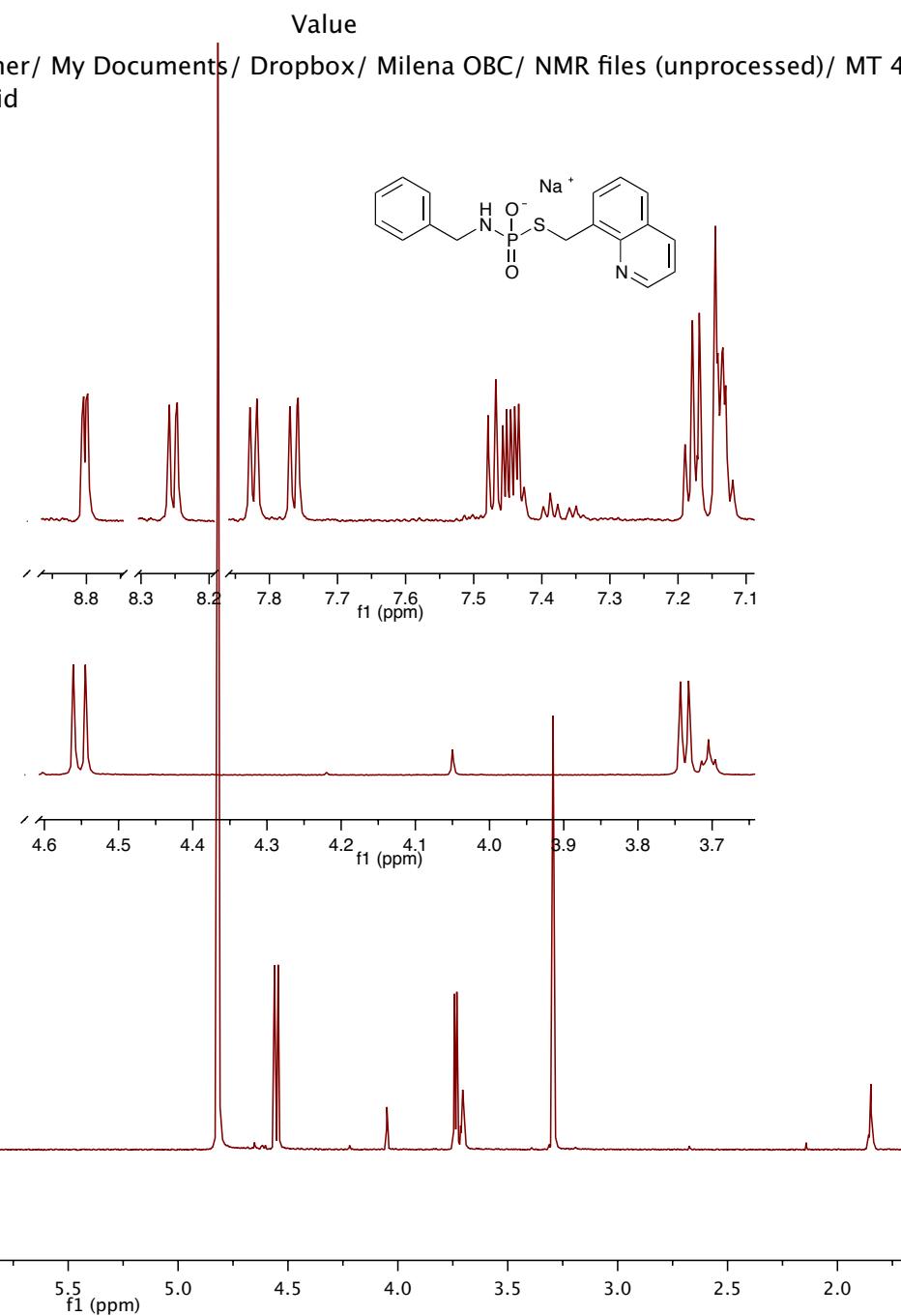
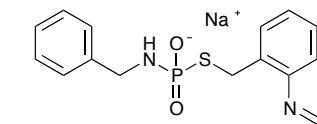
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Origin	Varian
Owner	
Site	
Spectrometer	vnmrs
Author	service
Solvent	cd3od
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	256
Receiver Gain	50
Relaxation Delay	3.0000
Pulse Width	0.0000
Acquisition Time	0.7340
Acquisition Date	2009-02-21T04:58:54
Modification Date	2012-04-23T11:56:53
Spectrometer Frequency	283.26
Spectral Width	44642.9
Lowest Frequency	-15919.8
Nucleus	31P
Acquired Size	32768
Spectral Size	65536



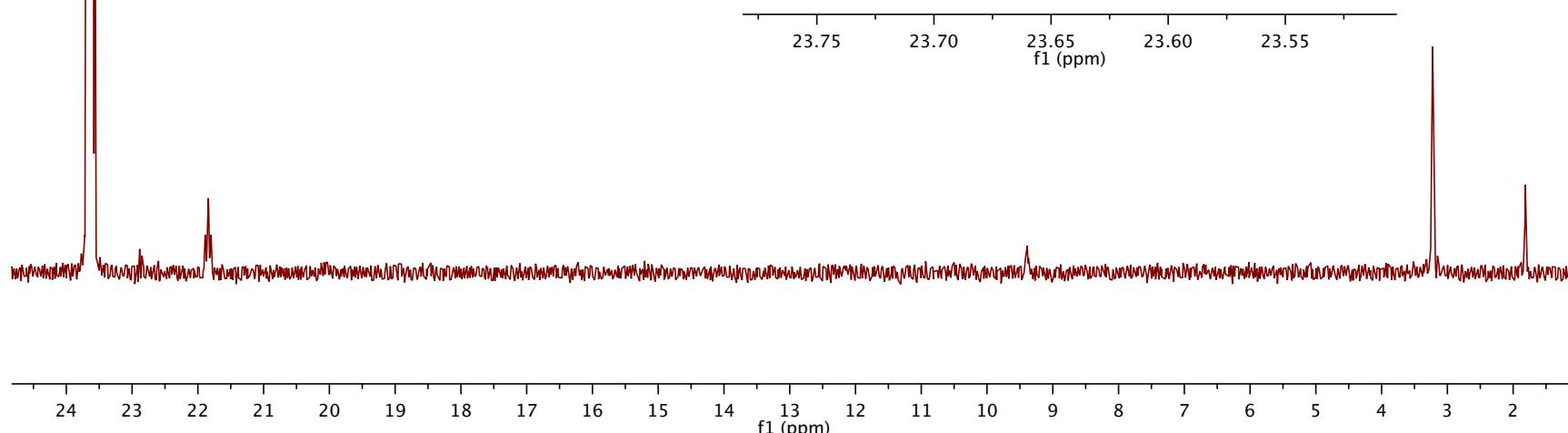
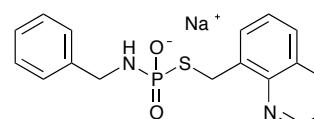
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10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	1000
13 Receiver Gain	60
14 Relaxation Delay	2.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.4680
17 Acquisition Date	2009-02-14T08:25:40
18 Modification Date	2012-11-06T16:58:51
19 Spectrometer Frequency	175.97
20 Spectral Width	44642.9
21 Lowest Frequency	-2967.2
22 Nucleus	¹³ C
23 Acquired Size	65536
24 Spectral Size	131072



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10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	4
13 Receiver Gain	42
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	2.9098
17 Acquisition Date	2009-02-14T08:24:59
18 Modification Date	2012-11-06T16:58:51
19 Spectrometer Frequency	699.74
20 Spectral Width	11261.3
21 Lowest Frequency	-1432.2
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536

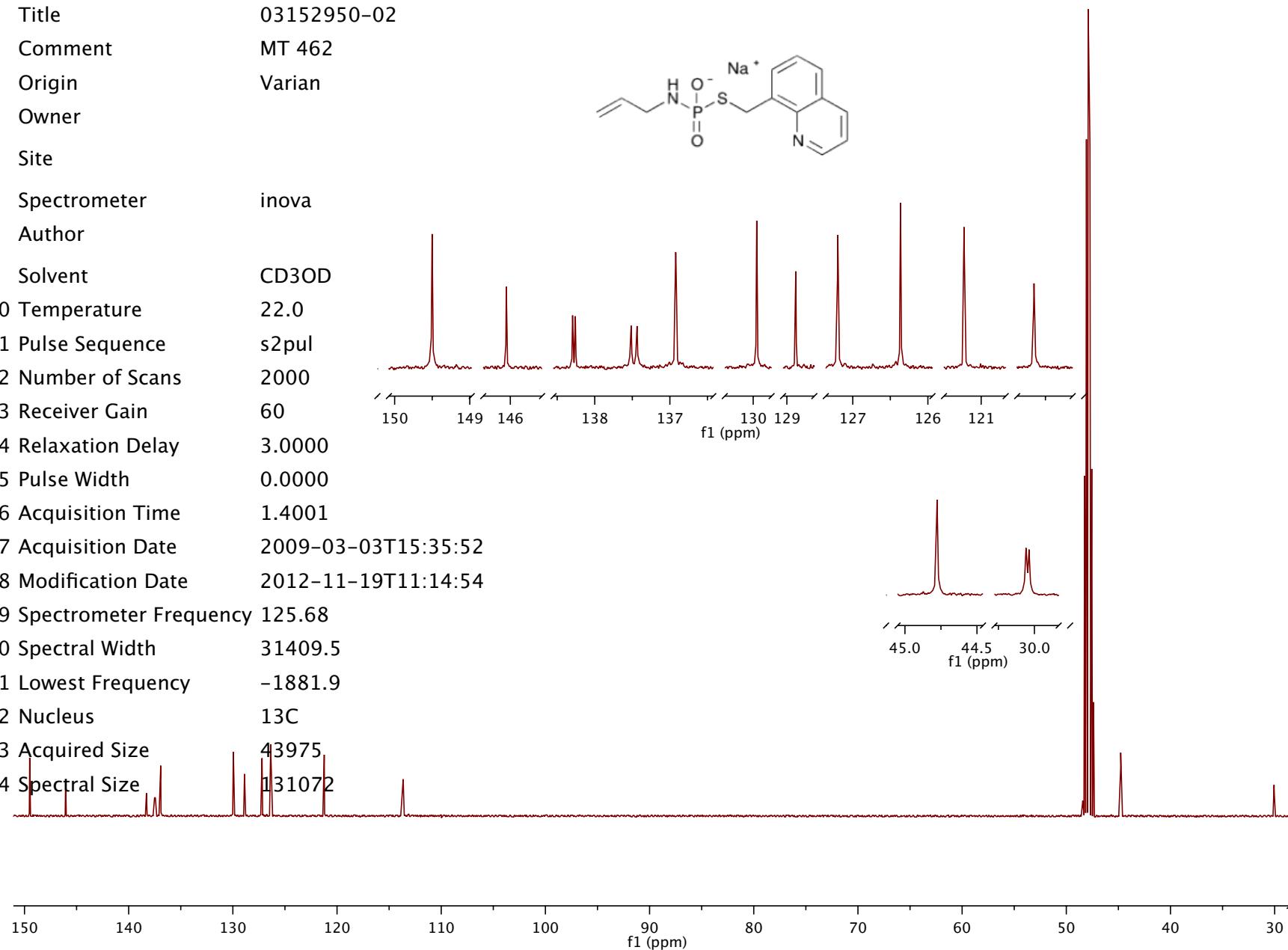
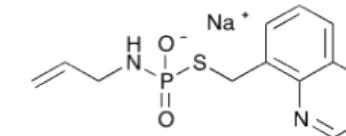


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3 Comment	MT 414
4 Origin	Varian
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7 Spectrometer	vnmrs
8 Author	service
9 Solvent	cd3od
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	256
13 Receiver Gain	50
14 Relaxation Delay	3.0000
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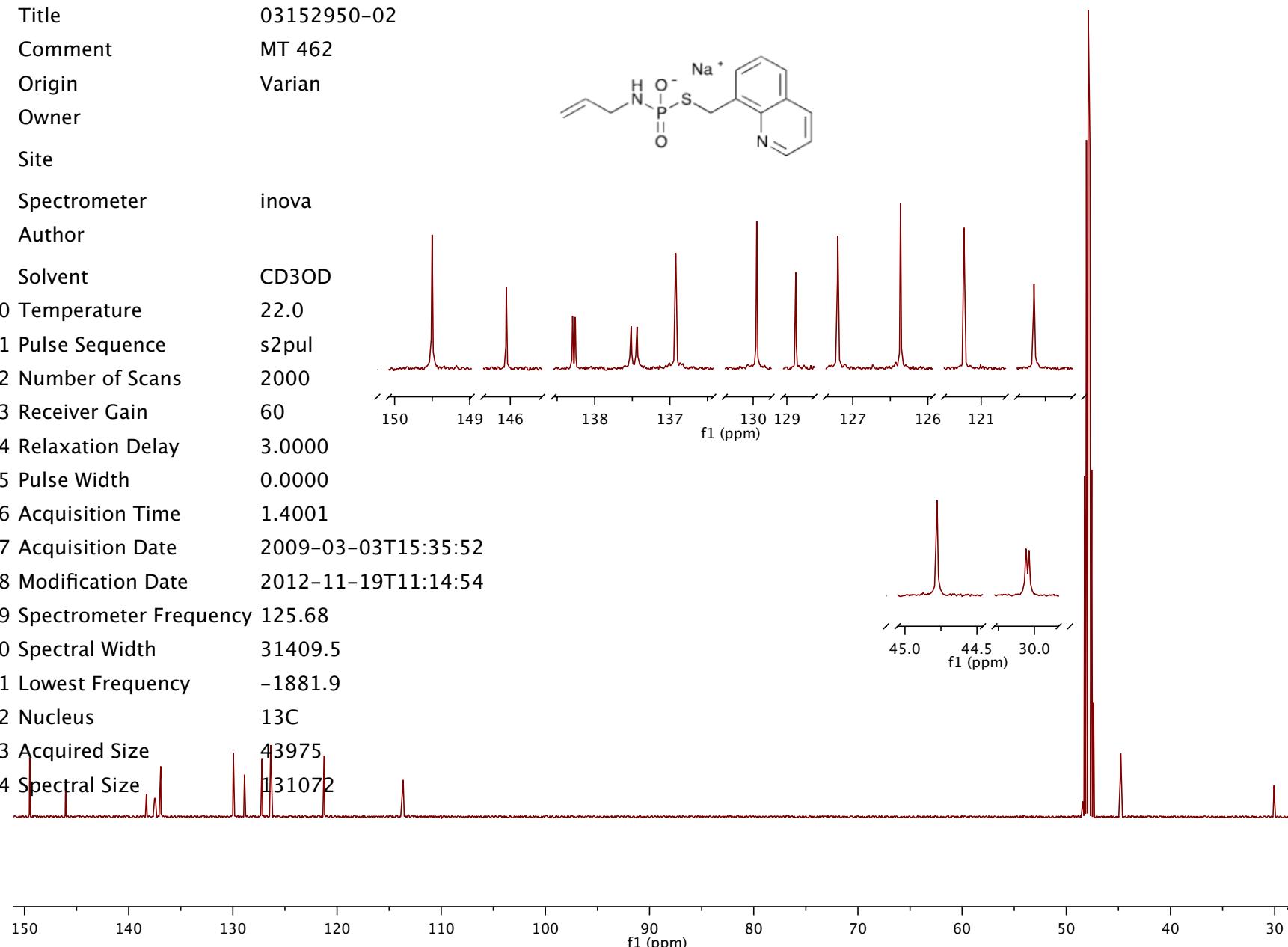
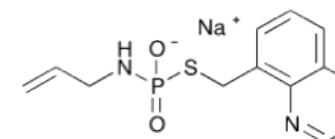
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4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	inova
8 Author	
9 Solvent	CD3OD
10 Temperature	22.0
11 Pulse Sequence	s2pul
12 Number of Scans	2000
13 Receiver Gain	60
14 Relaxation Delay	3.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.4001
17 Acquisition Date	2009-03-03T15:35:52
18 Modification Date	2012-11-19T11:14:54
19 Spectrometer Frequency	125.68
20 Spectral Width	31409.5
21 Lowest Frequency	-1881.9
22 Nucleus	¹³ C
23 Acquired Size	43975
24 Spectral Size	131072



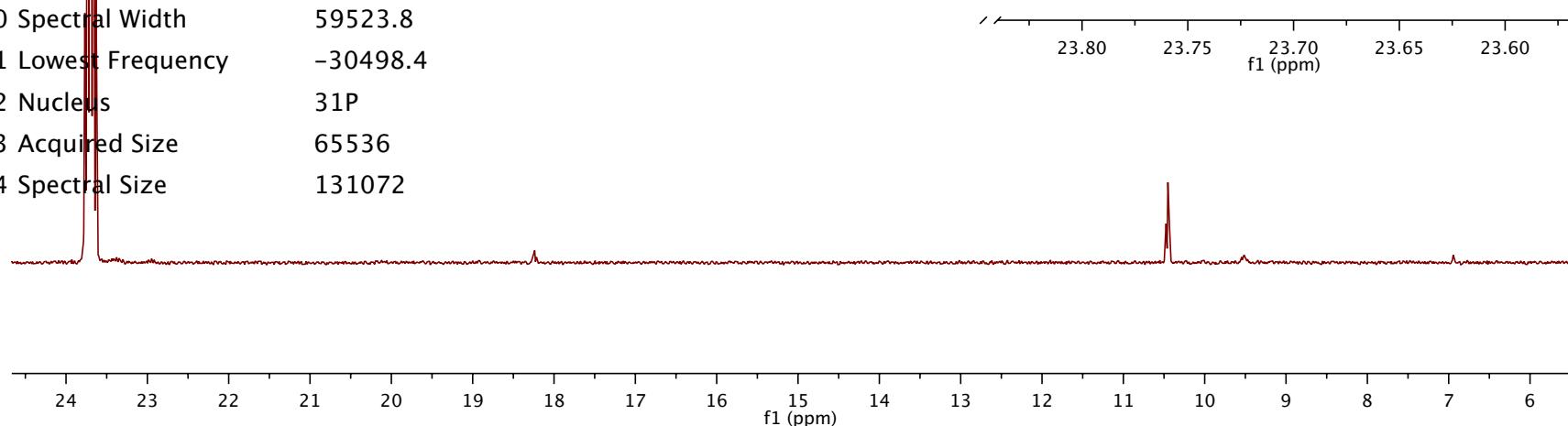
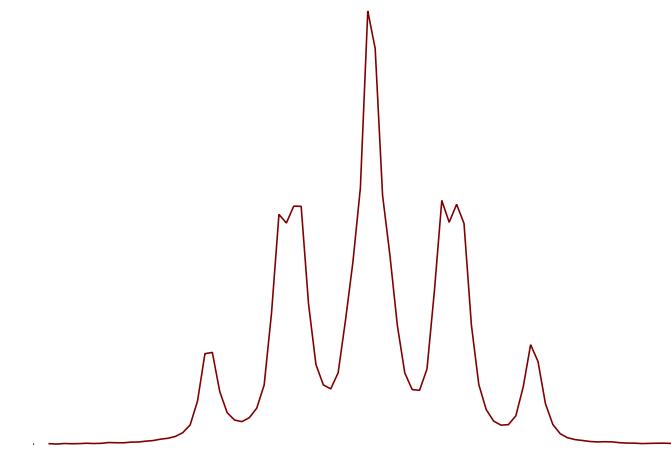
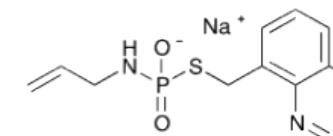
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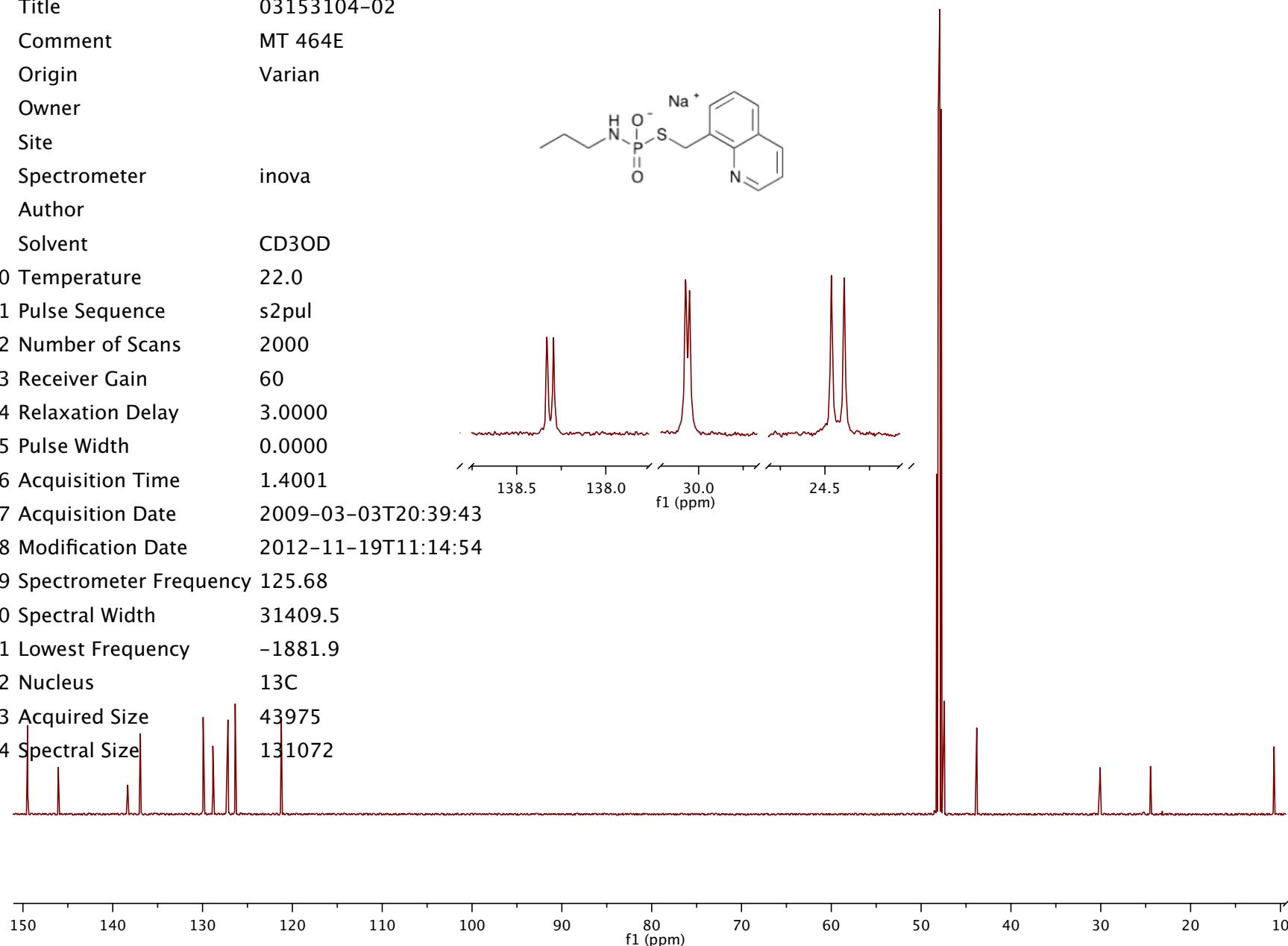
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5 Owner	
6 Site	
7 Spectrometer	inova
8 Author	
9 Solvent	CD3OD
10 Temperature	22.0
11 Pulse Sequence	s2pul
12 Number of Scans	2000
13 Receiver Gain	60
14 Relaxation Delay	3.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.4001
17 Acquisition Date	2009-03-03T15:35:52
18 Modification Date	2012-11-19T11:14:54
19 Spectrometer Frequency	125.68
20 Spectral Width	31409.5
21 Lowest Frequency	-1881.9
22 Nucleus	¹³ C
23 Acquired Size	43975
24 Spectral Size	131072



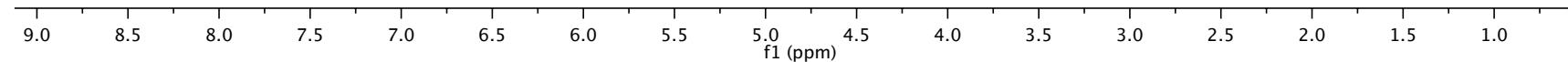
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4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	cd3od
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	256
13 Receiver Gain	50
14 Relaxation Delay	3.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.1010
17 Acquisition Date	2009-03-04T09:53:21
18 Modification Date	2012-11-19T11:11:20
19 Spectrometer Frequency	283.26
20 Spectral Width	59523.8
21 Lowest Frequency	-30498.4
22 Nucleus	³¹ P
23 Acquired Size	65536
24 Spectral Size	131072



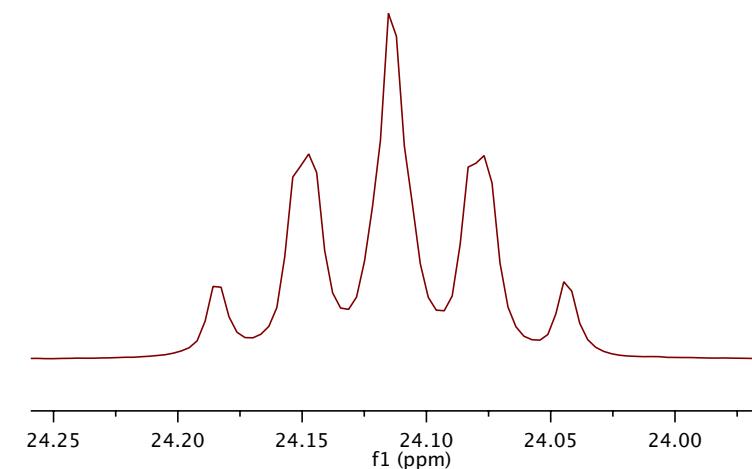
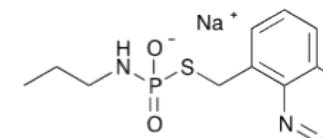
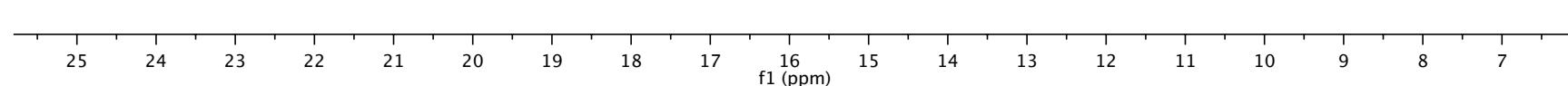
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4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	inova
8 Author	
9 Solvent	CD3OD
10 Temperature	22.0
11 Pulse Sequence	s2pul
12 Number of Scans	2000
13 Receiver Gain	60
14 Relaxation Delay	3.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.4001
17 Acquisition Date	2009-03-03T20:39:43
18 Modification Date	2012-11-19T11:14:54
19 Spectrometer Frequency	125.68
20 Spectral Width	31409.5
21 Lowest Frequency	-1881.9
22 Nucleus	¹³ C
23 Acquired Size	43975
24 Spectral Size	131072



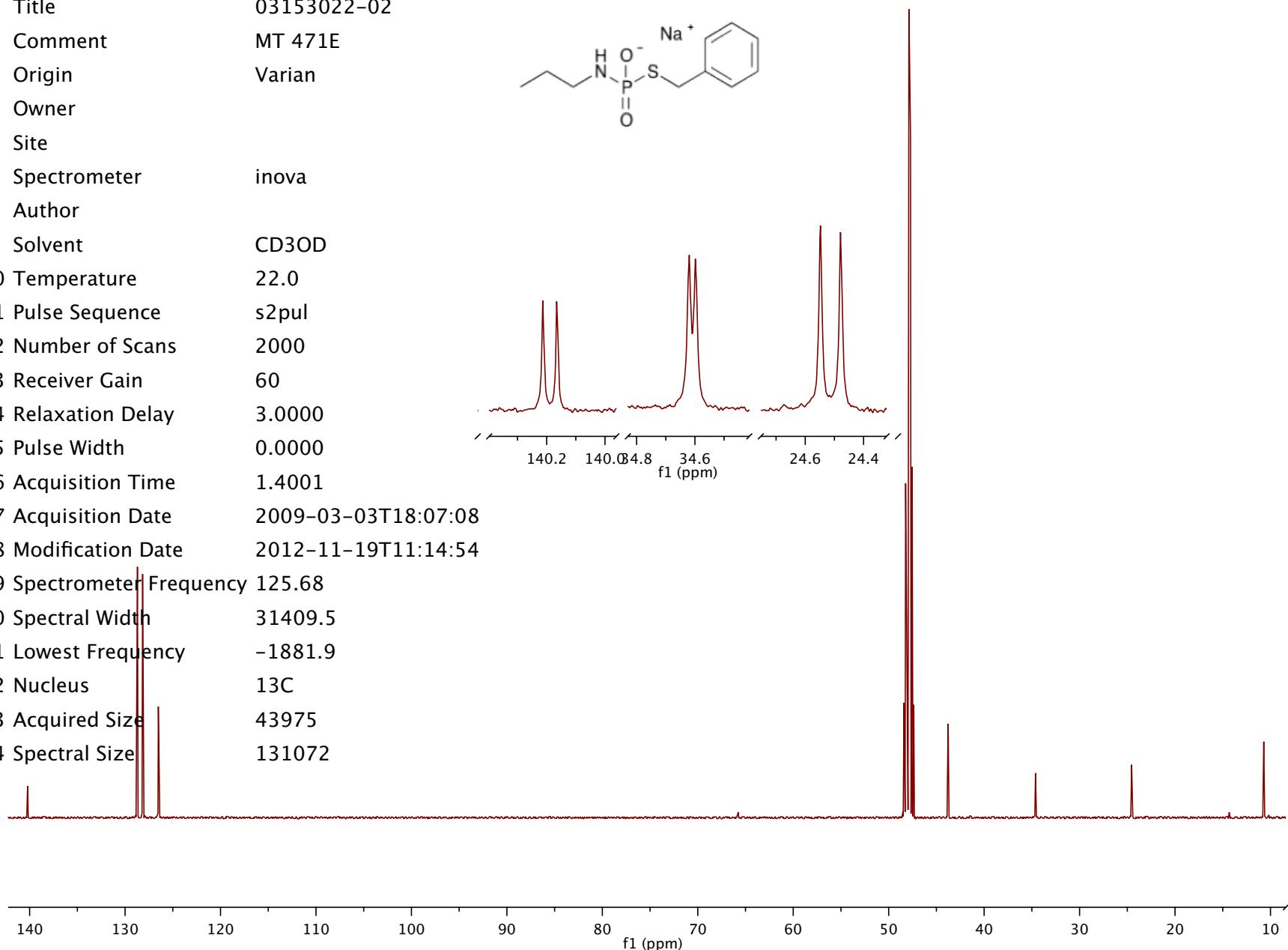
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4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	inova
8 Author	
9 Solvent	CD3OD
10 Temperature	29.0
11 Pulse Sequence	s2pul
12 Number of Scans	8
13 Receiver Gain	28
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	4.0000
17 Acquisition Date	2009-03-03T20:38:38
18 Modification Date	2012-11-06T17:41:00
19 Spectrometer Frequency	499.75
20 Spectral Width	7996.0
21 Lowest Frequency	-999.5
22 Nucleus	1H
23 Acquired Size	31984
24 Spectral Size	65536



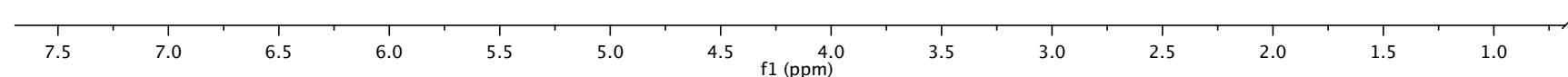
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7 Spectrometer	vnmrs
8 Author	service
9 Solvent	cd3od
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	256
13 Receiver Gain	50
14 Relaxation Delay	3.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.1010
17 Acquisition Date	2009-03-04T10:37:04
18 Modification Date	2012-11-06T17:40:23
19 Spectrometer Frequency	283.26
20 Spectral Width	59523.8
21 Lowest Frequency	-30498.4
22 Nucleus	^{31}P
23 Acquired Size	65536
24 Spectral Size	131072



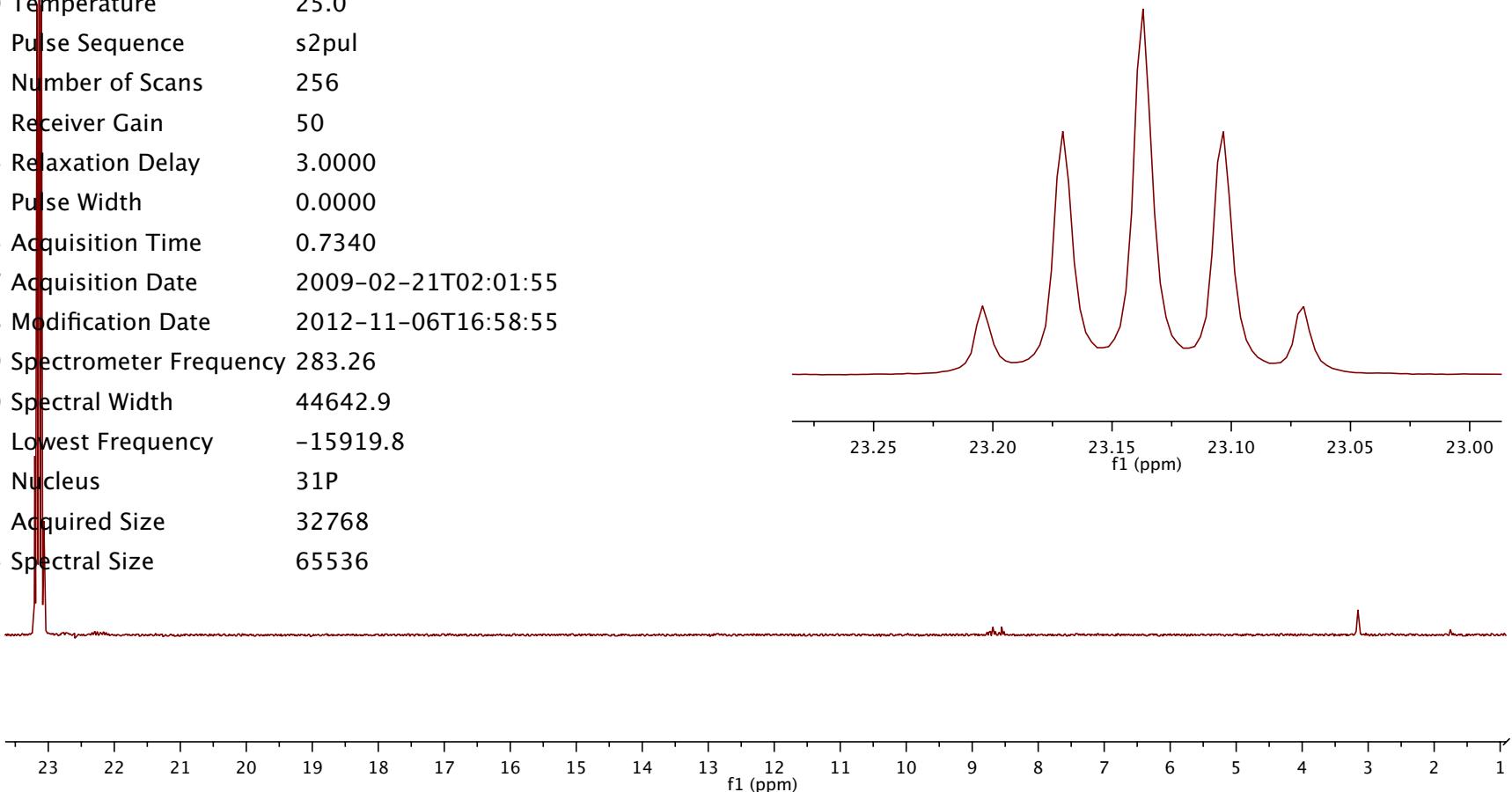
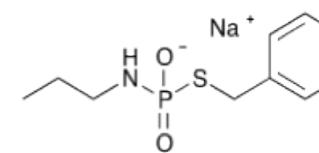
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4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	inova
8 Author	
9 Solvent	CD3OD
10 Temperature	22.0
11 Pulse Sequence	s2pul
12 Number of Scans	2000
13 Receiver Gain	60
14 Relaxation Delay	3.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.4001
17 Acquisition Date	2009-03-03T18:07:08
18 Modification Date	2012-11-19T11:14:54
19 Spectrometer Frequency	125.68
20 Spectral Width	31409.5
21 Lowest Frequency	-1881.9
22 Nucleus	¹³ C
23 Acquired Size	43975
24 Spectral Size	131072



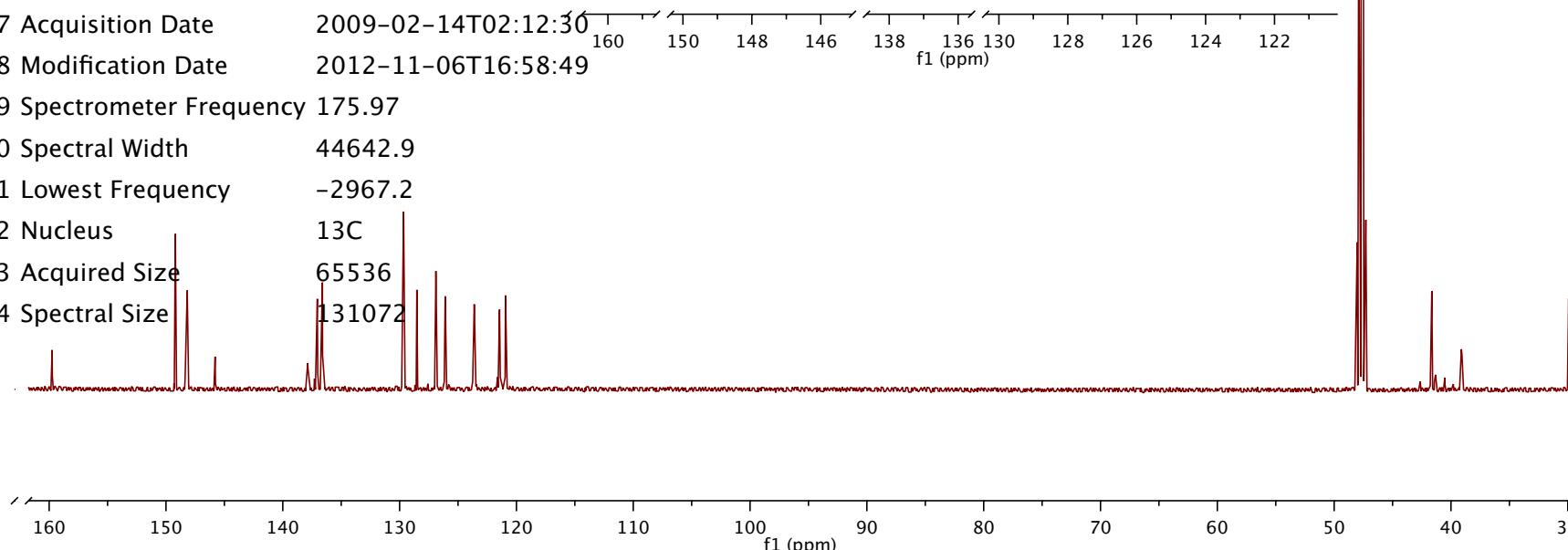
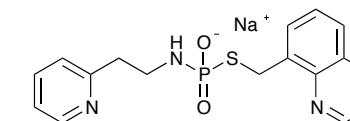
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7 Spectrometer	inova
8 Author	
9 Solvent	CD3OD
10 Temperature	29.0
11 Pulse Sequence	s2pul
12 Number of Scans	8
13 Receiver Gain	28
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	4.0000
17 Acquisition Date	2009-03-03T18:06:02
18 Modification Date	2012-11-19T11:14:54
19 Spectrometer Frequency	499.75
20 Spectral Width	7996.0
21 Lowest Frequency	-999.5
22 Nucleus	1H
23 Acquired Size	31984
24 Spectral Size	65536



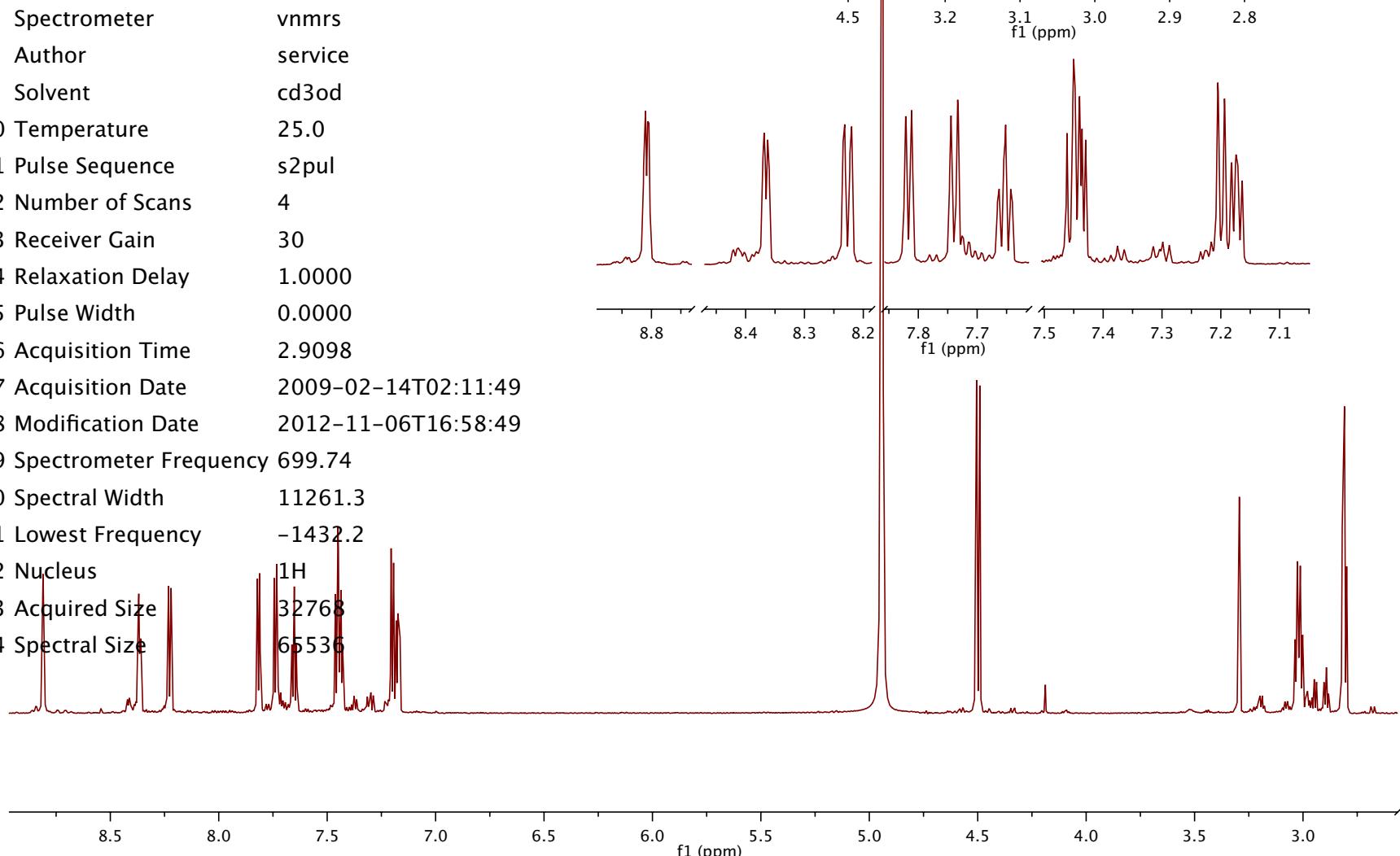
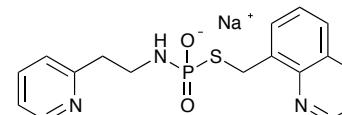
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6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	cd3od
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	256
13 Receiver Gain	50
14 Relaxation Delay	3.0000
15 Pulse Width	0.0000
16 Acquisition Time	0.7340
17 Acquisition Date	2009-02-21T02:01:55
18 Modification Date	2012-11-06T16:58:55
19 Spectrometer Frequency	283.26
20 Spectral Width	44642.9
21 Lowest Frequency	-15919.8
22 Nucleus	^{31}P
23 Acquired Size	32768
24 Spectral Size	65536



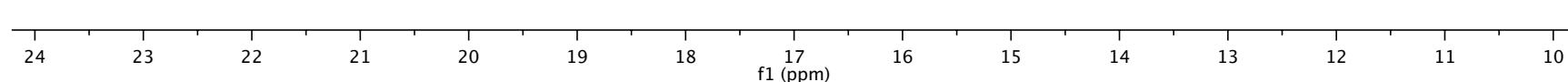
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6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	cd3od
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	1000
13 Receiver Gain	60
14 Relaxation Delay	2.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.4680
17 Acquisition Date	2009-02-14T02:12:30
18 Modification Date	2012-11-06T16:58:49
19 Spectrometer Frequency	175.97
20 Spectral Width	44642.9
21 Lowest Frequency	-2967.2
22 Nucleus	¹³ C
23 Acquired Size	65536
24 Spectral Size	131072



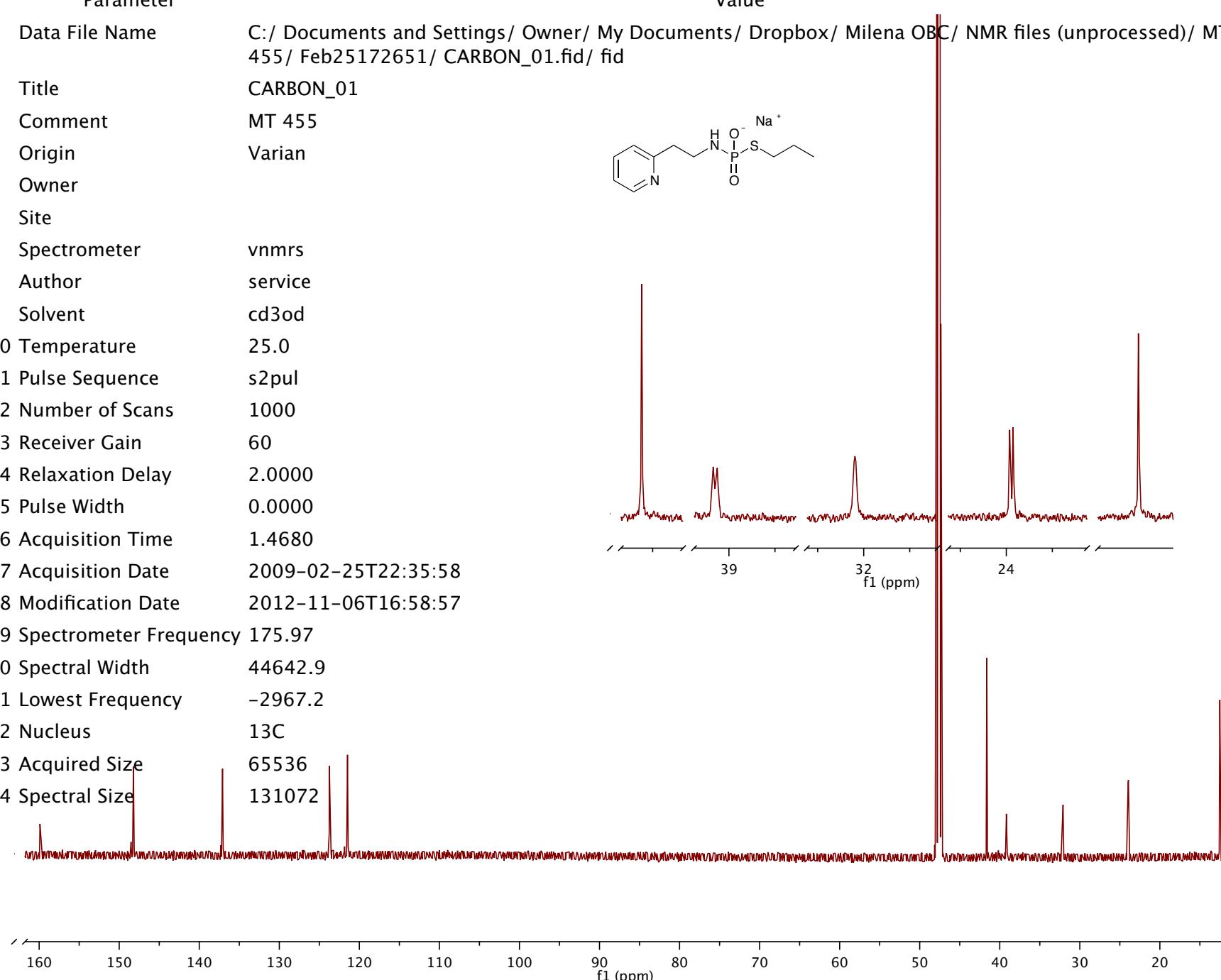
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8 Author	service
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10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	4
13 Receiver Gain	30
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	2.9098
17 Acquisition Date	2009-02-14T02:11:49
18 Modification Date	2012-11-06T16:58:49
19 Spectrometer Frequency	699.74
20 Spectral Width	11261.3
21 Lowest Frequency	-1432.2
22 Nucleus	¹ H
23 Acquired Size	32768
24 Spectral Size	65536



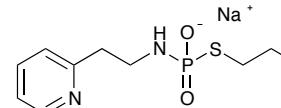
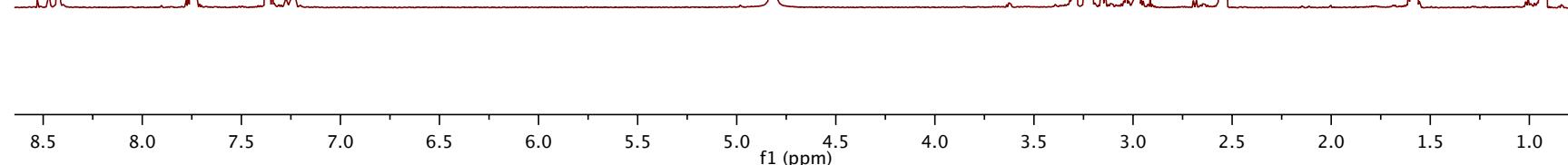
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6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	cd3od
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	256
13 Receiver Gain	50
14 Relaxation Delay	3.0000
15 Pulse Width	0.0000
16 Acquisition Time	0.7340
17 Acquisition Date	2009-02-20T19:51:19
18 Modification Date	2012-11-06T16:58:53
19 Spectrometer Frequency	283.26
20 Spectral Width	44642.9
21 Lowest Frequency	-15919.8
22 Nucleus	³¹ P
23 Acquired Size	32768
24 Spectral Size	65536



Parameter	Value
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6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	cd3od
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	1000
13 Receiver Gain	60
14 Relaxation Delay	2.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.4680
17 Acquisition Date	2009-02-25T22:35:58
18 Modification Date	2012-11-06T16:58:57
19 Spectrometer Frequency	175.97
20 Spectral Width	44642.9
21 Lowest Frequency	-2967.2
22 Nucleus	¹³ C
23 Acquired Size	65536
24 Spectral Size	131072



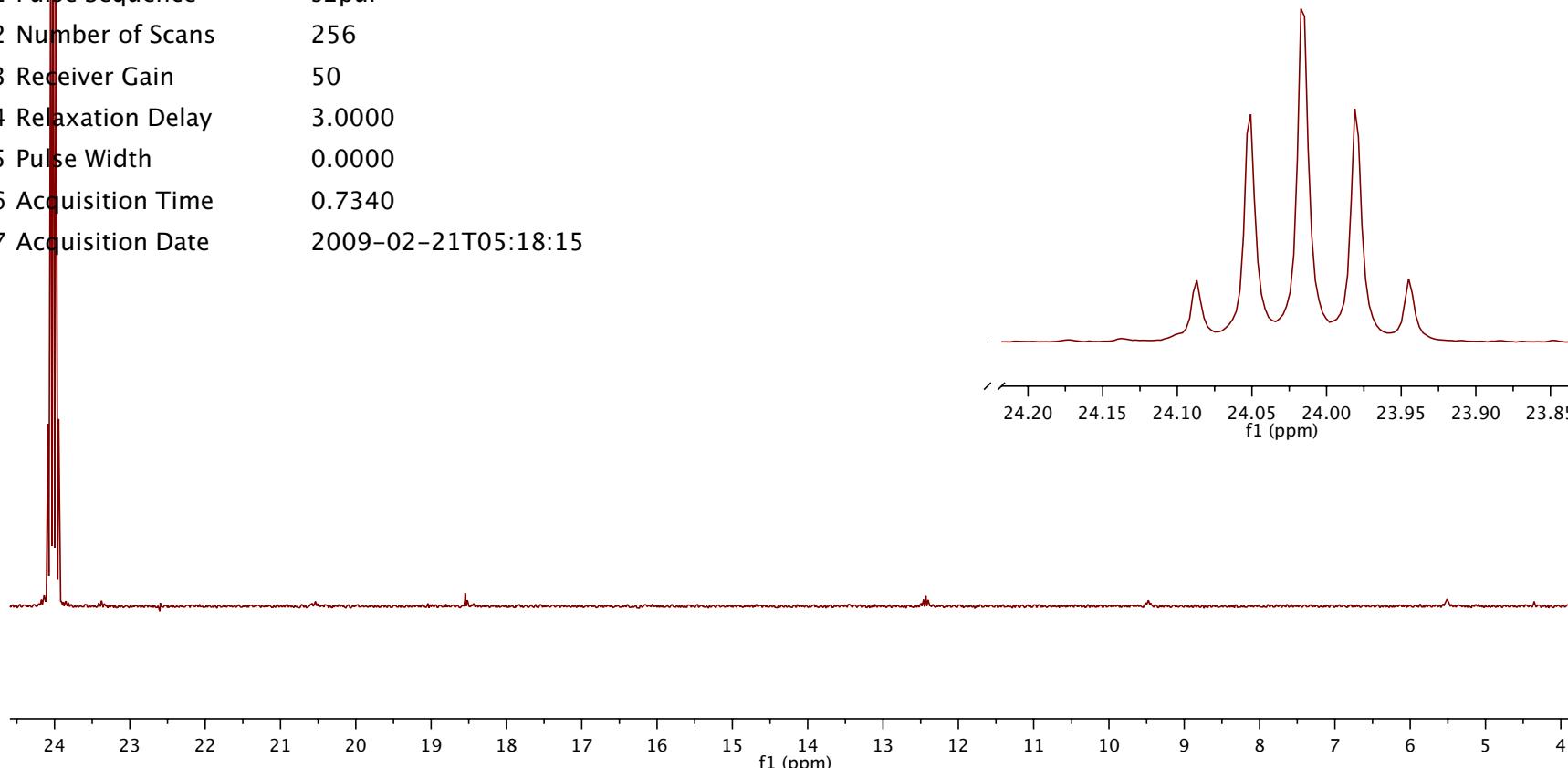
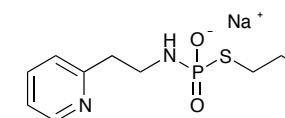
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3 Comment	MT 455
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	cd3od
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	4
13 Receiver Gain	30
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	2.9098
17 Acquisition Date	2009-02-25T22:35:18
18 Modification Date	2012-11-06T16:58:57
19 Spectrometer Frequency	699.74
20 Spectral Width	11261.3
21 Lowest Frequency	-1432.2
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536



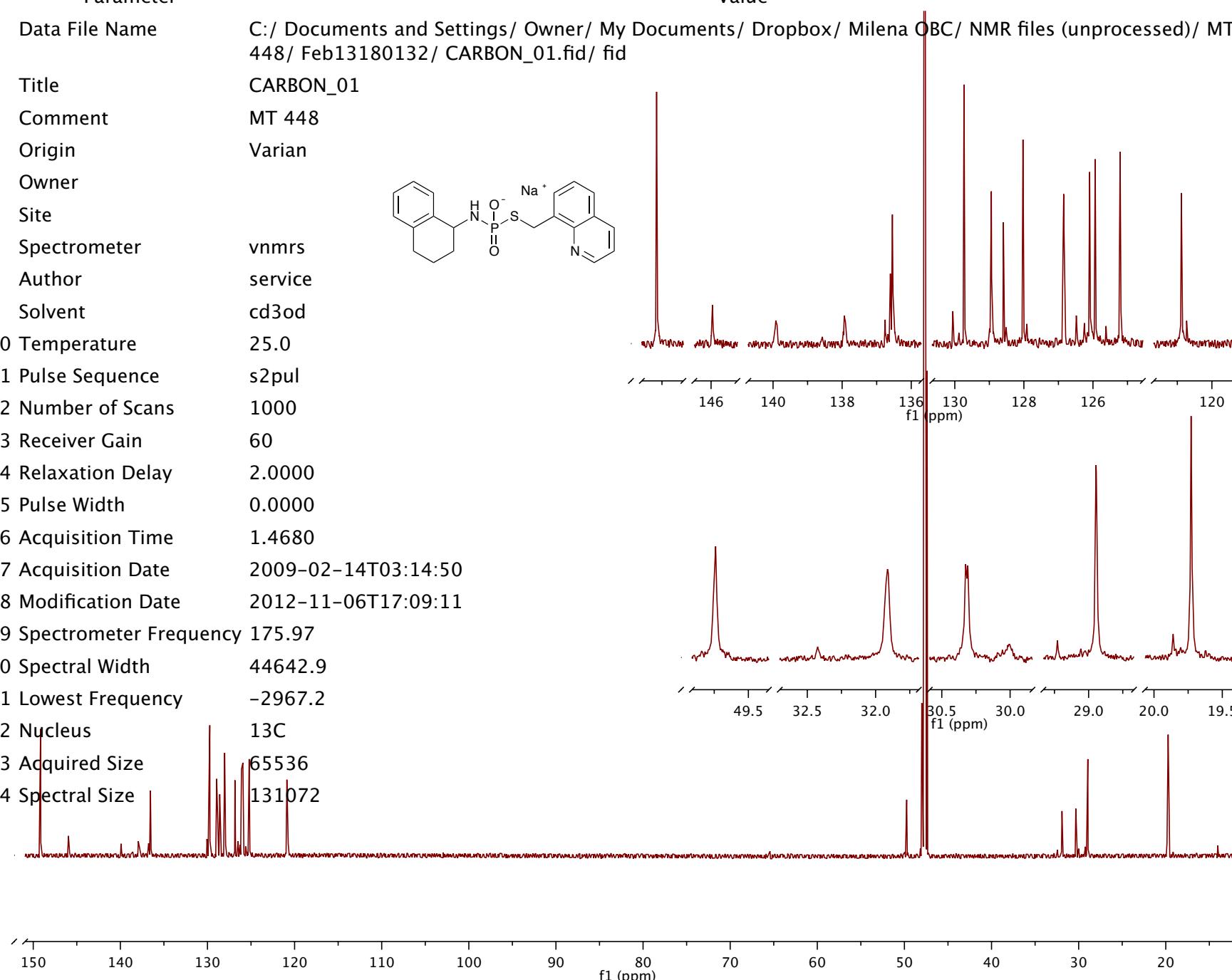
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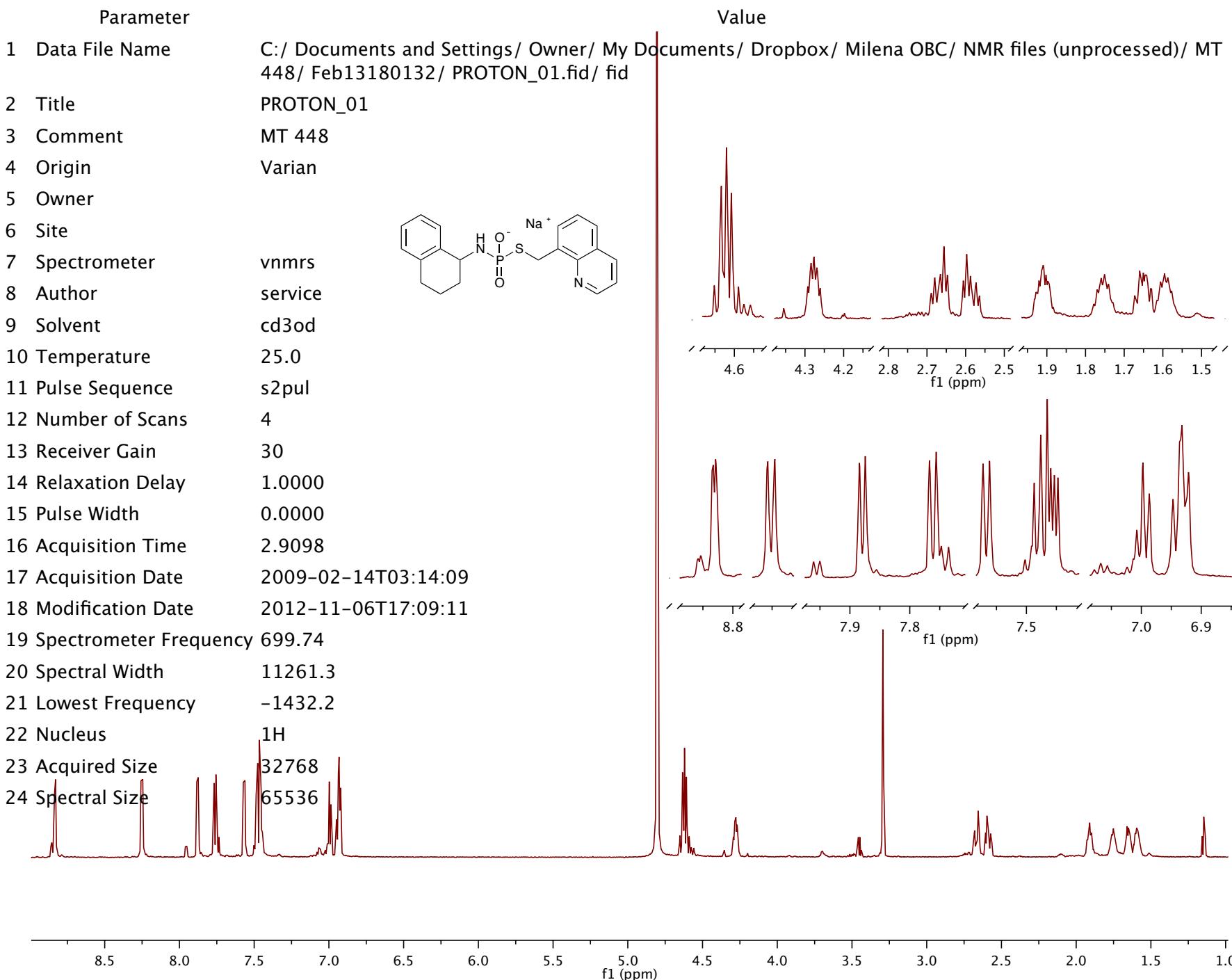
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5	Owner	
6	Site	
7	Spectrometer	vnmrs
8	Author	service
9	Solvent	cd3od
10	Temperature	25.0
11	Pulse Sequence	s2pul
12	Number of Scans	256
13	Receiver Gain	50
14	Relaxation Delay	3.0000
15	Pulse Width	0.0000
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17	Acquisition Date	2009-02-21T05:18:15

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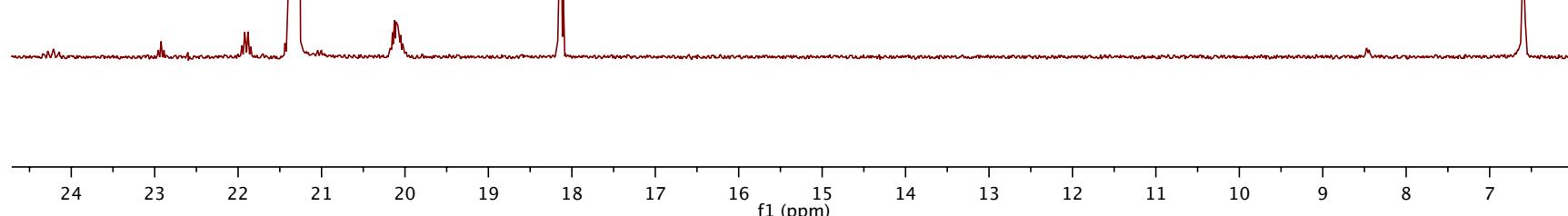


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4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	cd3od
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	1000
13 Receiver Gain	60
14 Relaxation Delay	2.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.4680
17 Acquisition Date	2009-02-14T03:14:50
18 Modification Date	2012-11-06T17:09:11
19 Spectrometer Frequency	175.97
20 Spectral Width	44642.9
21 Lowest Frequency	-2967.2
22 Nucleus	¹³ C
23 Acquired Size	65536
24 Spectral Size	131072

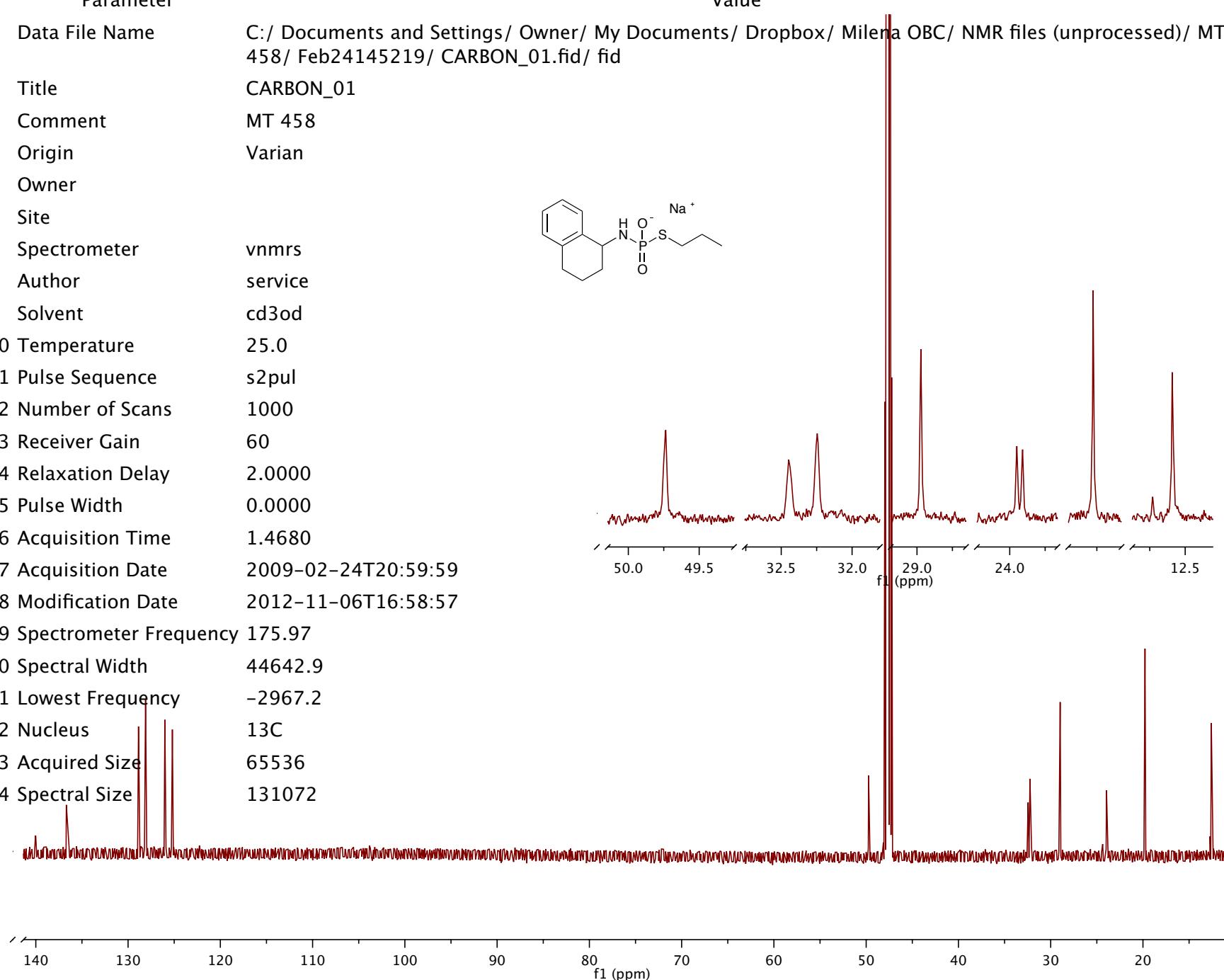


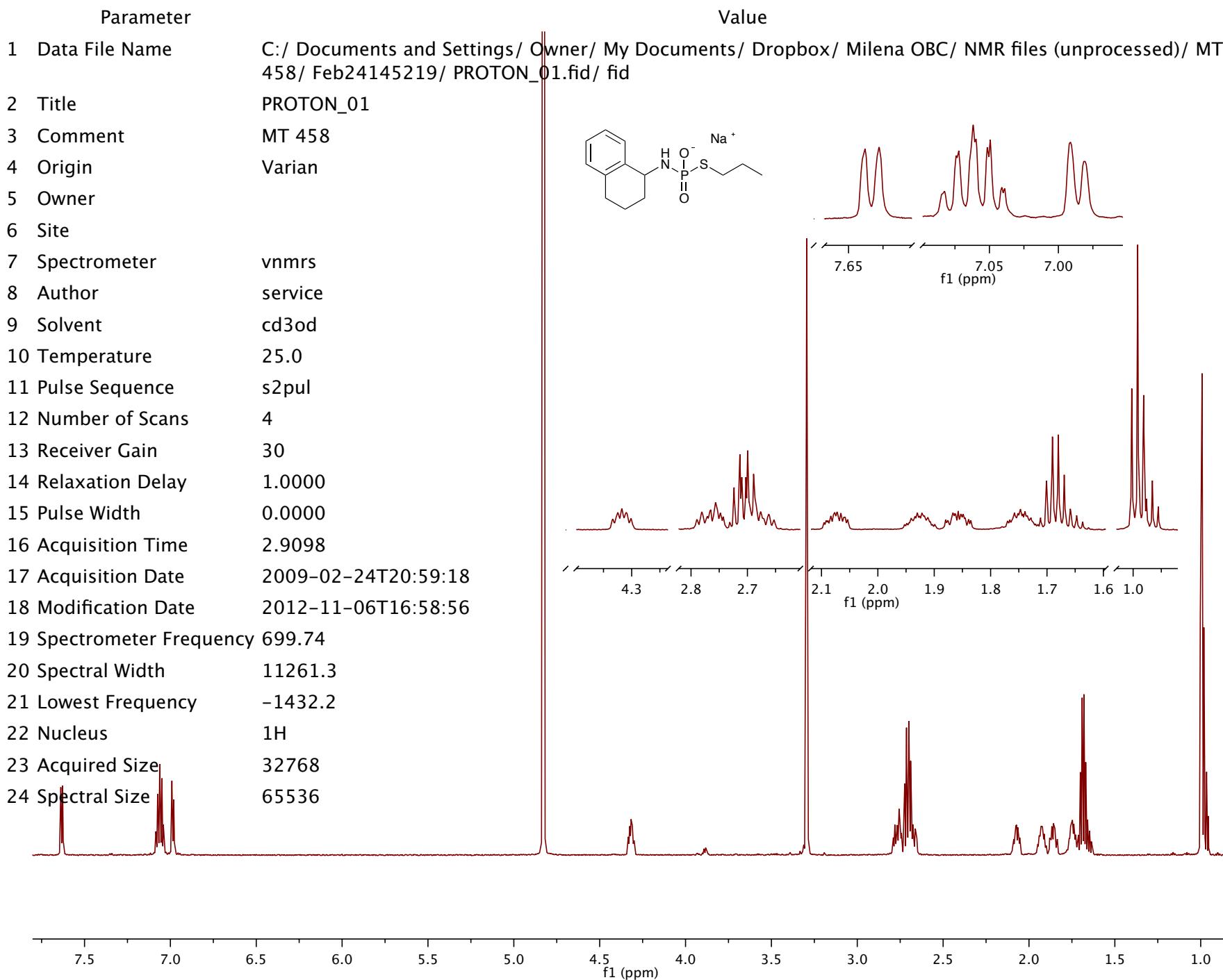


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2 Title	PHOSPHORUS_01
3 Comment	MT 448
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	cd3od
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	256
13 Receiver Gain	50
14 Relaxation Delay	3.0000
15 Pulse Width	0.0000
16 Acquisition Time	0.7340
17 Acquisition Date	2009-02-20T20:30:11
18 Modification Date	2012-11-06T16:58:54
19 Spectrometer Frequency	283.26
20 Spectral Width	44642.9
21 Lowest Frequency	-15919.8
22 Nucleus	³¹ P
23 Acquired Size	32768
24 Spectral Size	65536



Parameter	Value
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3 Comment	MT 458
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5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	cd3od
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	1000
13 Receiver Gain	60
14 Relaxation Delay	2.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.4680
17 Acquisition Date	2009-02-24T20:59:59
18 Modification Date	2012-11-06T16:58:57
19 Spectrometer Frequency	175.97
20 Spectral Width	44642.9
21 Lowest Frequency	-2967.2
22 Nucleus	¹³ C
23 Acquired Size	65536
24 Spectral Size	131072

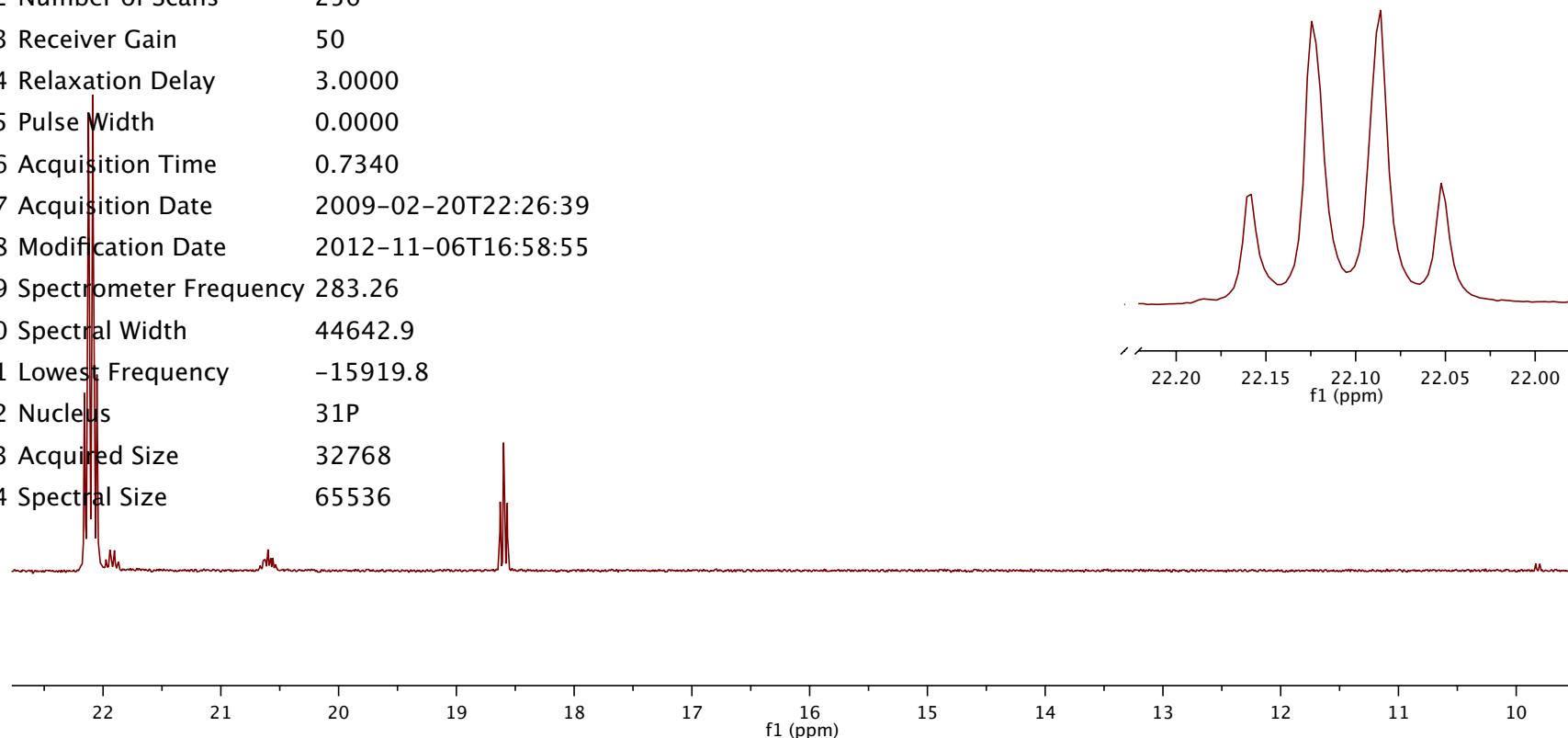
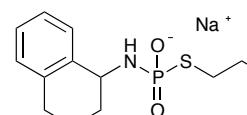




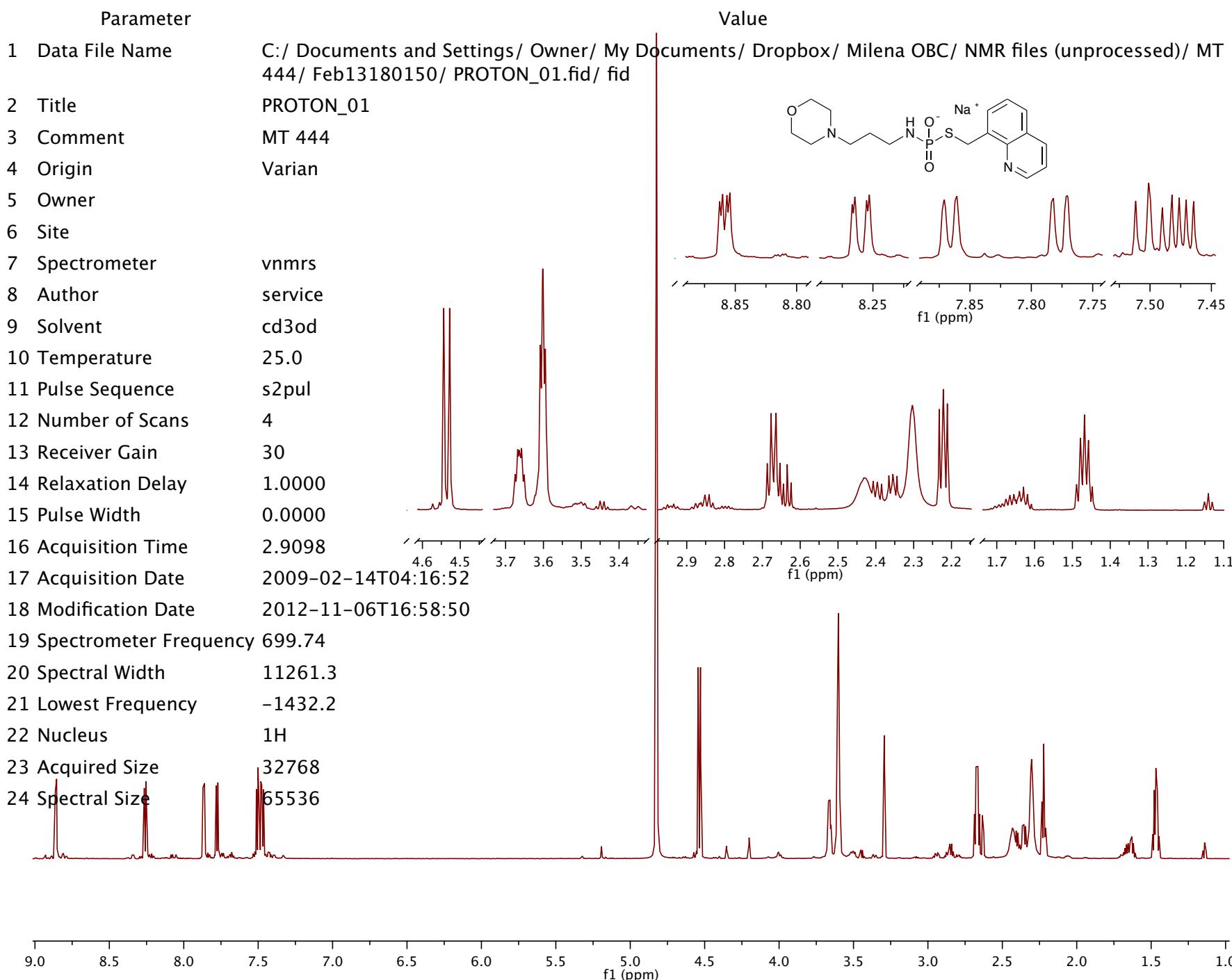
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3 Comment	MT 458
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	cd3od
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	256
13 Receiver Gain	50
14 Relaxation Delay	3.0000
15 Pulse Width	0.0000
16 Acquisition Time	0.7340
17 Acquisition Date	2009-02-20T22:26:39
18 Modification Date	2012-11-06T16:58:55
19 Spectrometer Frequency	283.26
20 Spectral Width	44642.9
21 Lowest Frequency	-15919.8
22 Nucleus	³¹ P
23 Acquired Size	32768
24 Spectral Size	65536



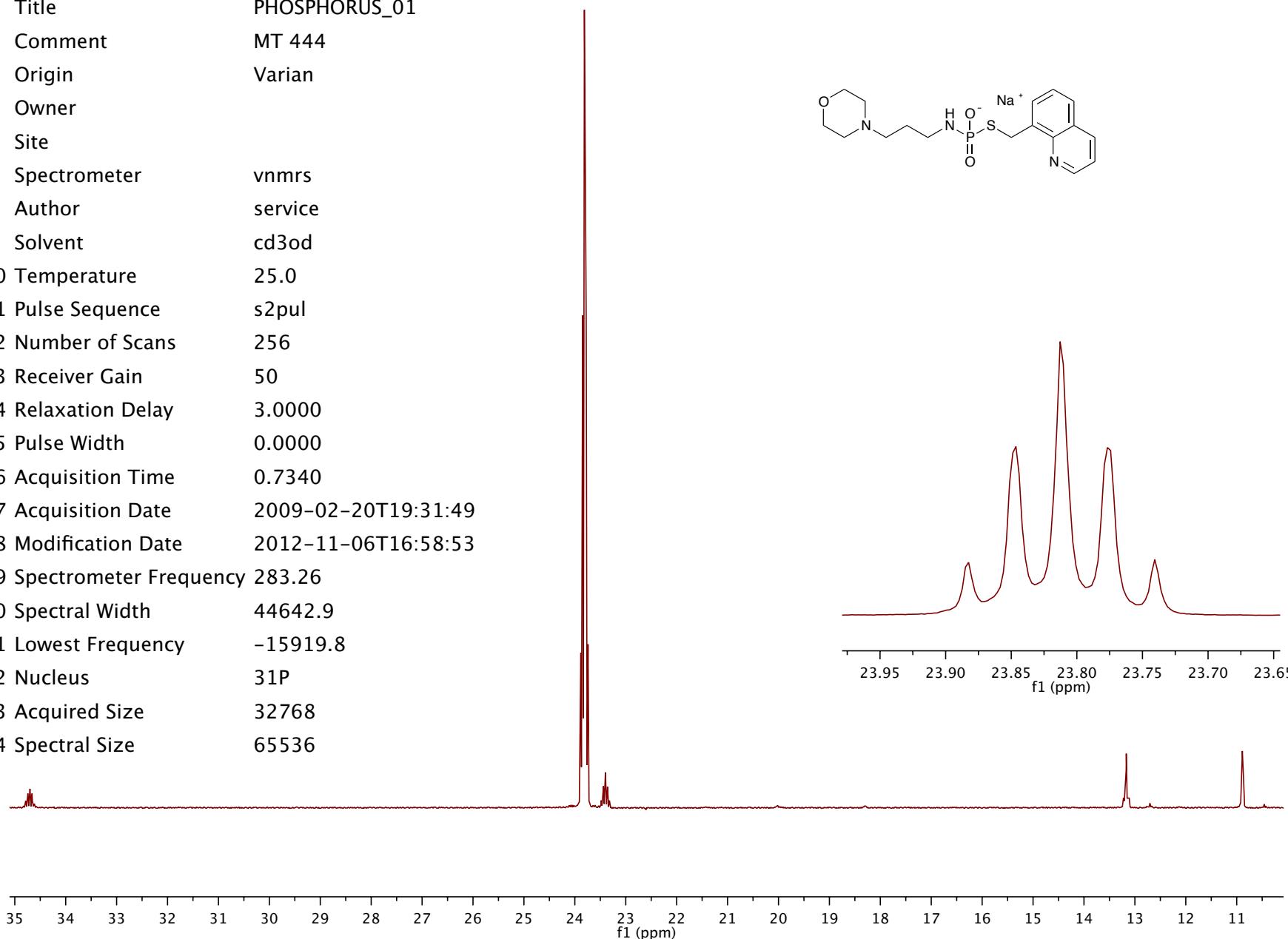
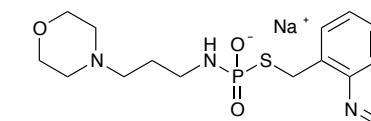
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5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	cd3od
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	1000
13 Receiver Gain	60
14 Relaxation Delay	2.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.4680
17 Acquisition Date	2009-02-14T04:17:34
18 Modification Date	2012-11-06T16:58:50
19 Spectrometer Frequency	175.97
20 Spectral Width	44642.9
21 Lowest Frequency	-2967.2
22 Nucleus	¹³ C
23 Acquired Size	65536
24 Spectral Size	131072



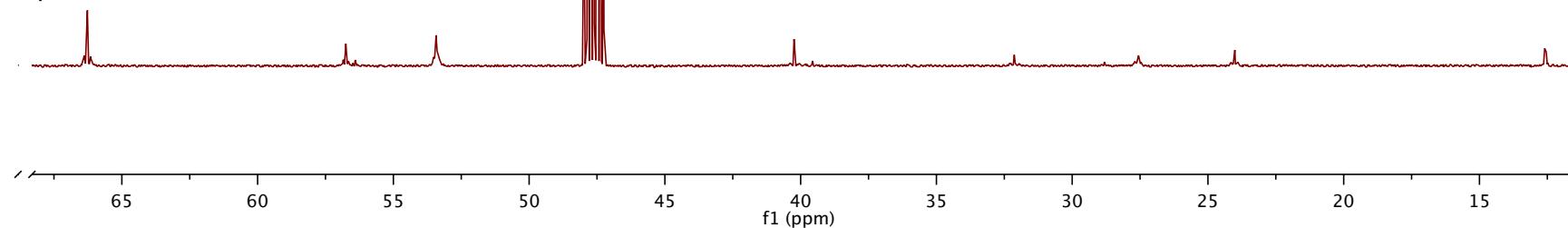
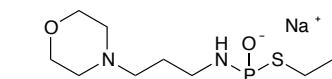
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5	Owner	
6	Site	
7	Spectrometer	vnmrs
8	Author	service
9	Solvent	cd3od
10	Temperature	25.0
11	Pulse Sequence	s2pul
12	Number of Scans	256
13	Receiver Gain	50
14	Relaxation Delay	3.0000
15	Pulse Width	0.0000
16	Acquisition Time	0.7340
17	Acquisition Date	2009-02-20T19:31:49
18	Modification Date	2012-11-06T16:58:53
19	Spectrometer Frequency	283.26
20	Spectral Width	44642.9
21	Lowest Frequency	-15919.8
22	Nucleus	31P
23	Acquired Size	32768
24	Spectral Size	65536

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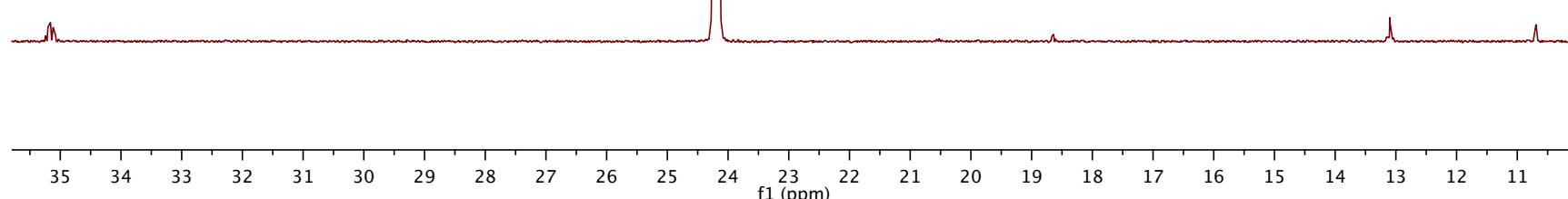


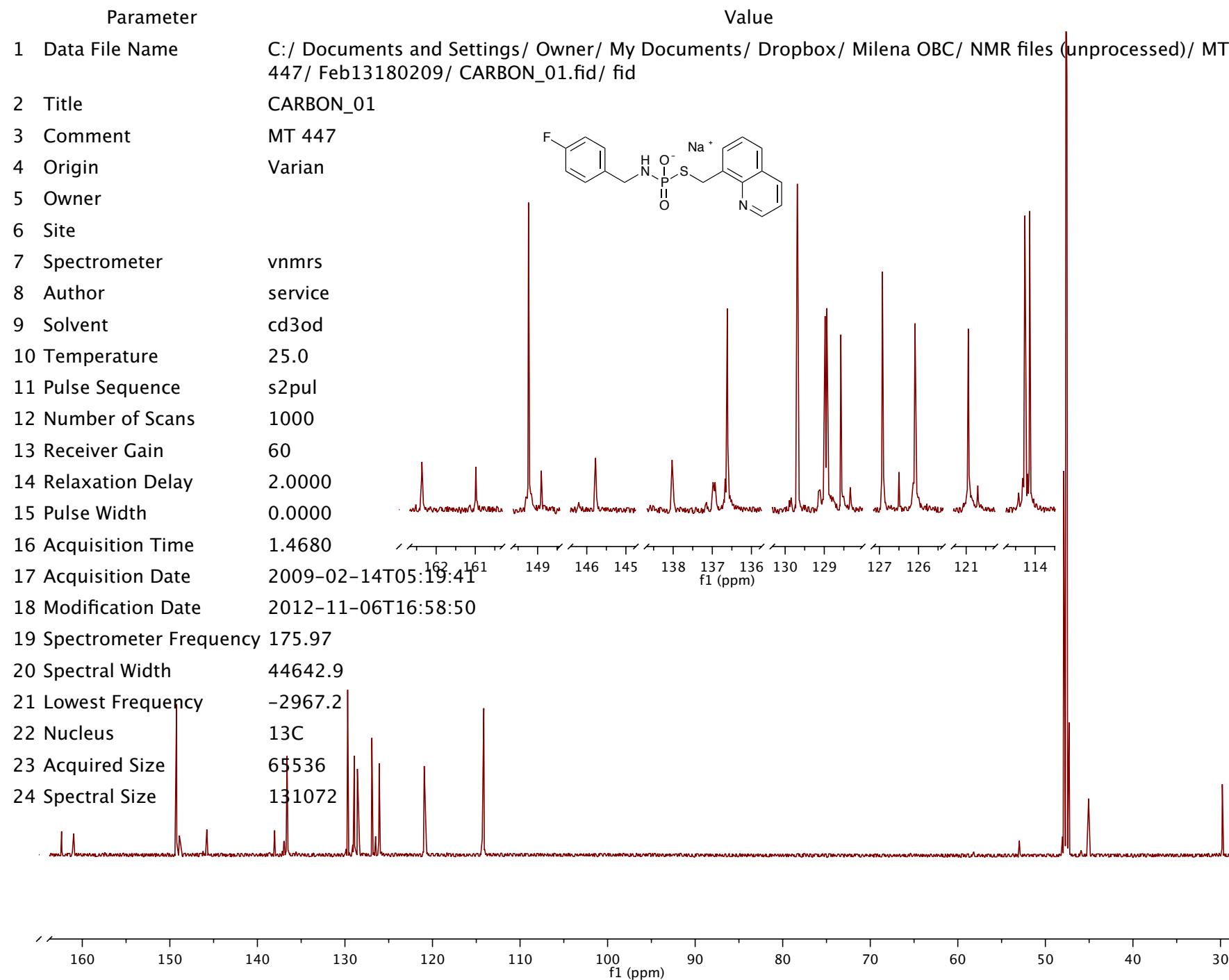
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3 Comment	MT 454
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	cd3od
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	1000
13 Receiver Gain	60
14 Relaxation Delay	2.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.4680
17 Acquisition Date	2009-02-16T21:06:33
18 Modification Date	2012-11-06T17:23:47
19 Spectrometer Frequency	175.97
20 Spectral Width	44642.9
21 Lowest Frequency	-2967.2
22 Nucleus	¹³ C
23 Acquired Size	65536
24 Spectral Size	131072



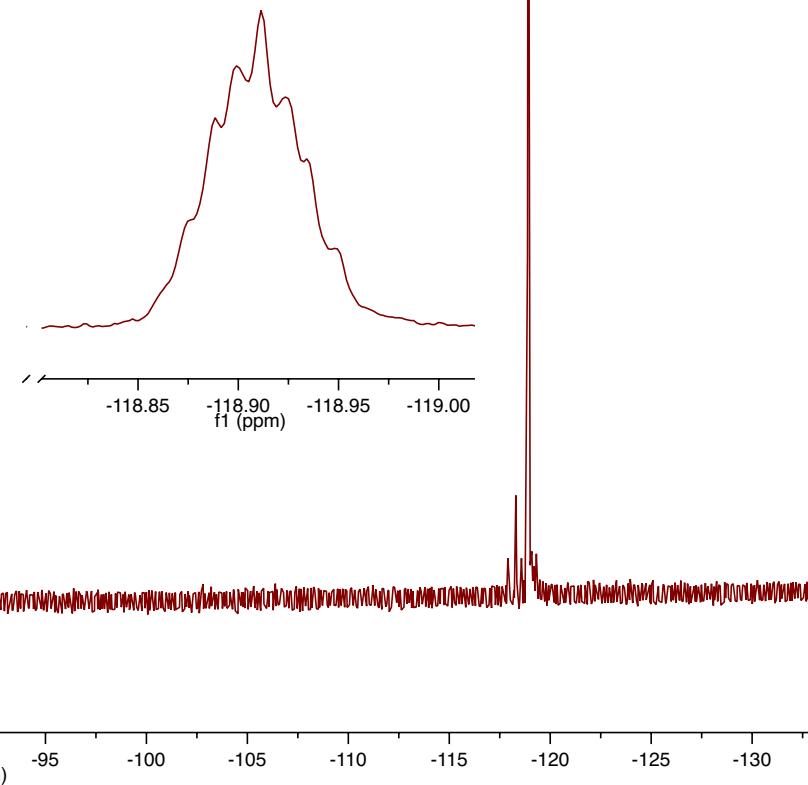
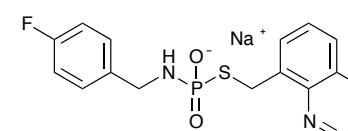
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3 Comment	MT 454
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	cd3od
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	4
13 Receiver Gain	30
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	2.9098
17 Acquisition Date	2009-02-16T21:05:52
18 Modification Date	2012-11-06T17:23:47
19 Spectrometer Frequency	699.74
20 Spectral Width	11261.3
21 Lowest Frequency	-1432.2
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536

Parameter	Value
1 Data File Name	C:/ Documents and Settings/ Owner/ My Documents/ Dropbox/ Milena OBC/ NMR files (unprocessed)/ MT454/ Feb20170506/ PHOSPHORUS_01.fid/ fid
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3 Comment	MT 454
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	cd3od
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	256
13 Receiver Gain	50
14 Relaxation Delay	3.0000
15 Pulse Width	0.0000
16 Acquisition Time	0.7340
17 Acquisition Date	2009-02-21T01:42:20
18 Modification Date	2012-11-06T16:58:55
19 Spectrometer Frequency	283.26
20 Spectral Width	44642.9
21 Lowest Frequency	-15919.8
22 Nucleus	^{31}P
23 Acquired Size	32768
24 Spectral Size	65536

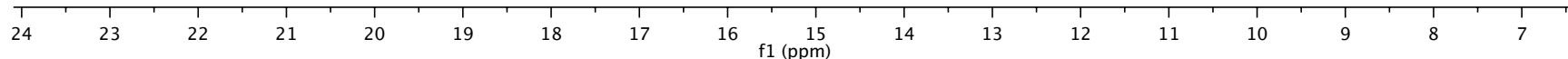




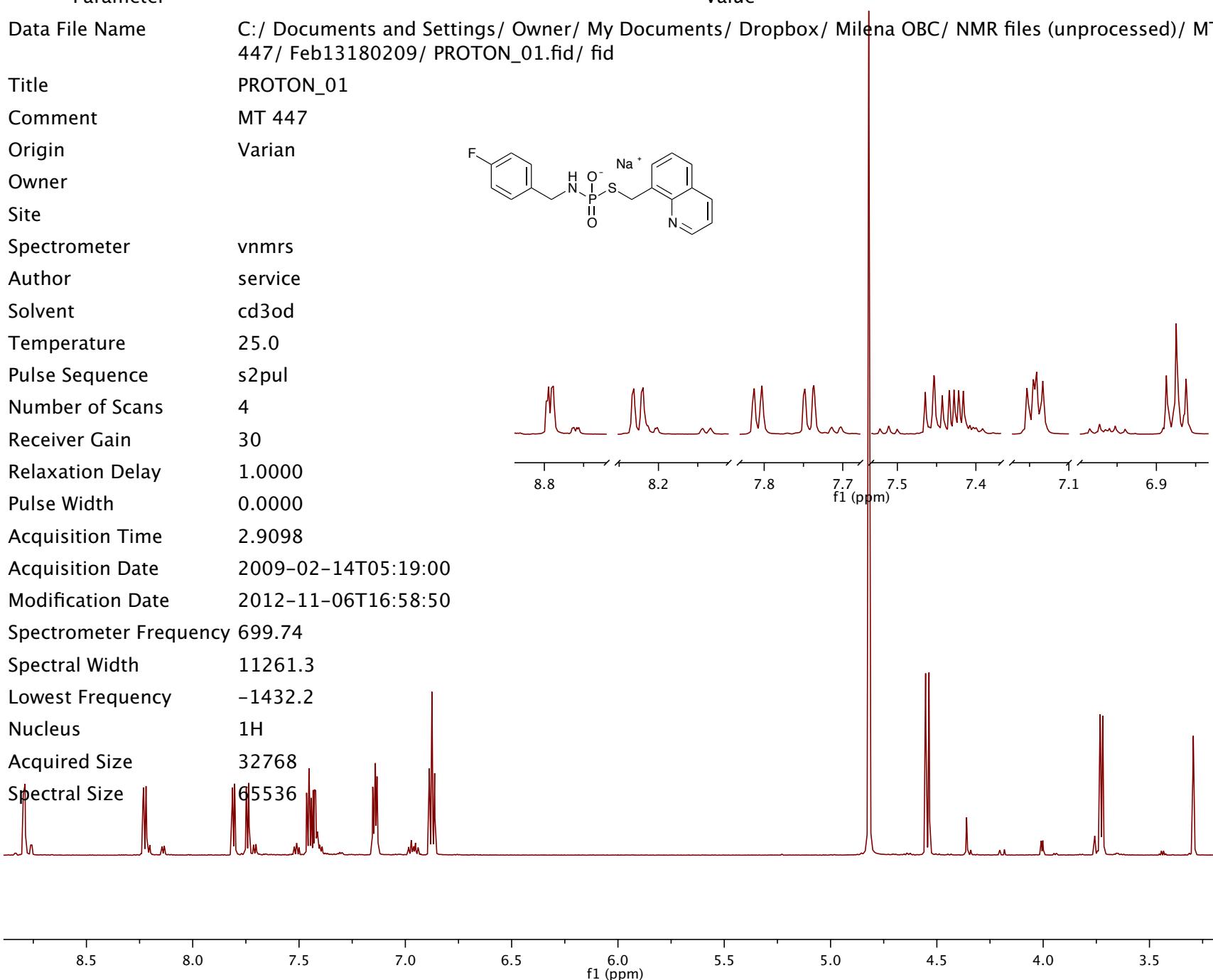
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4 Origin	Bruker BioSpin GmbH
5 Owner	Administrator
6 Site	
7 Spectrometer	av400
8 Author	
9 Solvent	MeOD
10 Temperature	293.4
11 Pulse Sequence	zgflqn
12 Number of Scans	16
13 Receiver Gain	912
14 Relaxation Delay	2.0000
15 Pulse Width	11.8000
16 Acquisition Time	0.8717
17 Acquisition Date	2009-05-11T14:19:00
18 Modification Date	2012-11-06T17:27:40
19 Spectrometer Frequency	376.39
20 Spectral Width	75188.0
21 Lowest Frequency	-71472.1
22 Nucleus	19F
23 Acquired Size	65536
24 Comments	



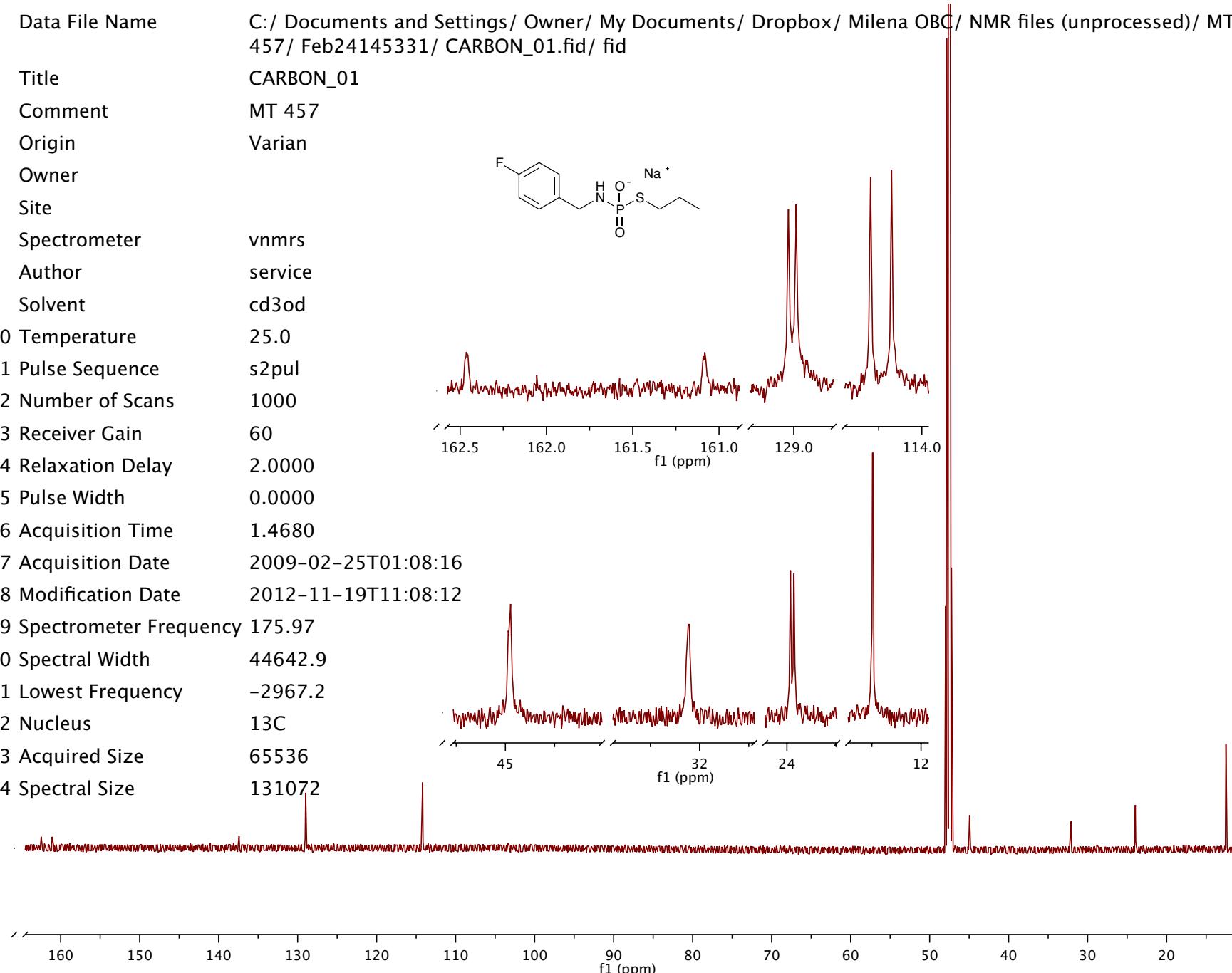
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3 Comment	MT 447
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	cd3od
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	256
13 Receiver Gain	50
14 Relaxation Delay	3.0000
15 Pulse Width	0.0000
16 Acquisition Time	0.7340
17 Acquisition Date	2009-02-20T20:10:45
18 Modification Date	2012-11-06T16:58:54
19 Spectrometer Frequency	283.26
20 Spectral Width	44642.9
21 Lowest Frequency	-15919.8
22 Nucleus	³¹ P
23 Acquired Size	32768
24 Spectral Size	65536



Parameter	Value
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4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	cd3od
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	4
13 Receiver Gain	30
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	2.9098
17 Acquisition Date	2009-02-14T05:19:00
18 Modification Date	2012-11-06T16:58:50
19 Spectrometer Frequency	699.74
20 Spectral Width	11261.3
21 Lowest Frequency	-1432.2
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536



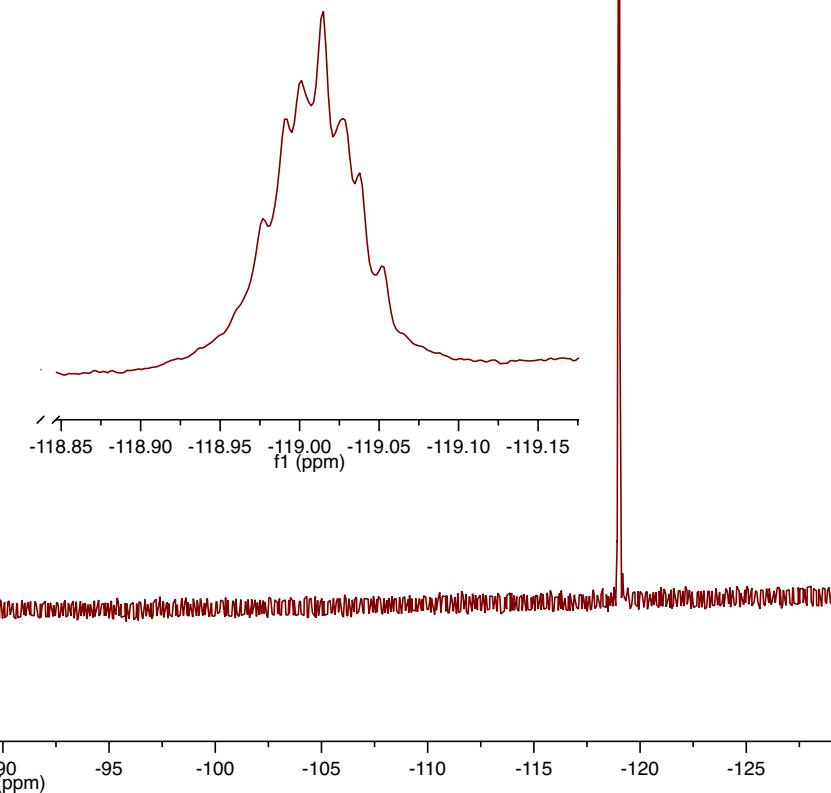
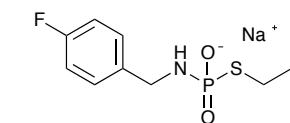
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4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	cd3od
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	1000
13 Receiver Gain	60
14 Relaxation Delay	2.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.4680
17 Acquisition Date	2009-02-25T01:08:16
18 Modification Date	2012-11-19T11:08:12
19 Spectrometer Frequency	175.97
20 Spectral Width	44642.9
21 Lowest Frequency	-2967.2
22 Nucleus	¹³ C
23 Acquired Size	65536
24 Spectral Size	131072



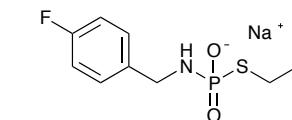
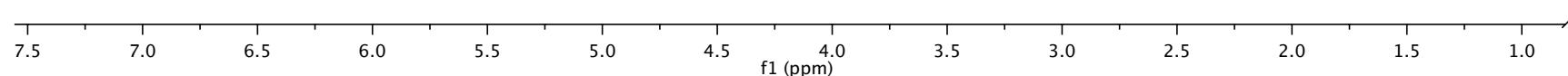
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4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	av400
8	Author	
9	Solvent	MeOD
10	Temperature	293.4
11	Pulse Sequence	zgflqn
12	Number of Scans	16
13	Receiver Gain	645
14	Relaxation Delay	2.0000
15	Pulse Width	11.8000
16	Acquisition Time	0.8717
17	Acquisition Date	2009-05-11T14:27:00
18	Modification Date	2012-11-06T17:28:03
19	Spectrometer Frequency	376.39
20	Spectral Width	75188.0
21	Lowest Frequency	-71472.1
22	Nucleus	19F
23	Acquired Size	65536
24	Spectral Size	131072

Value



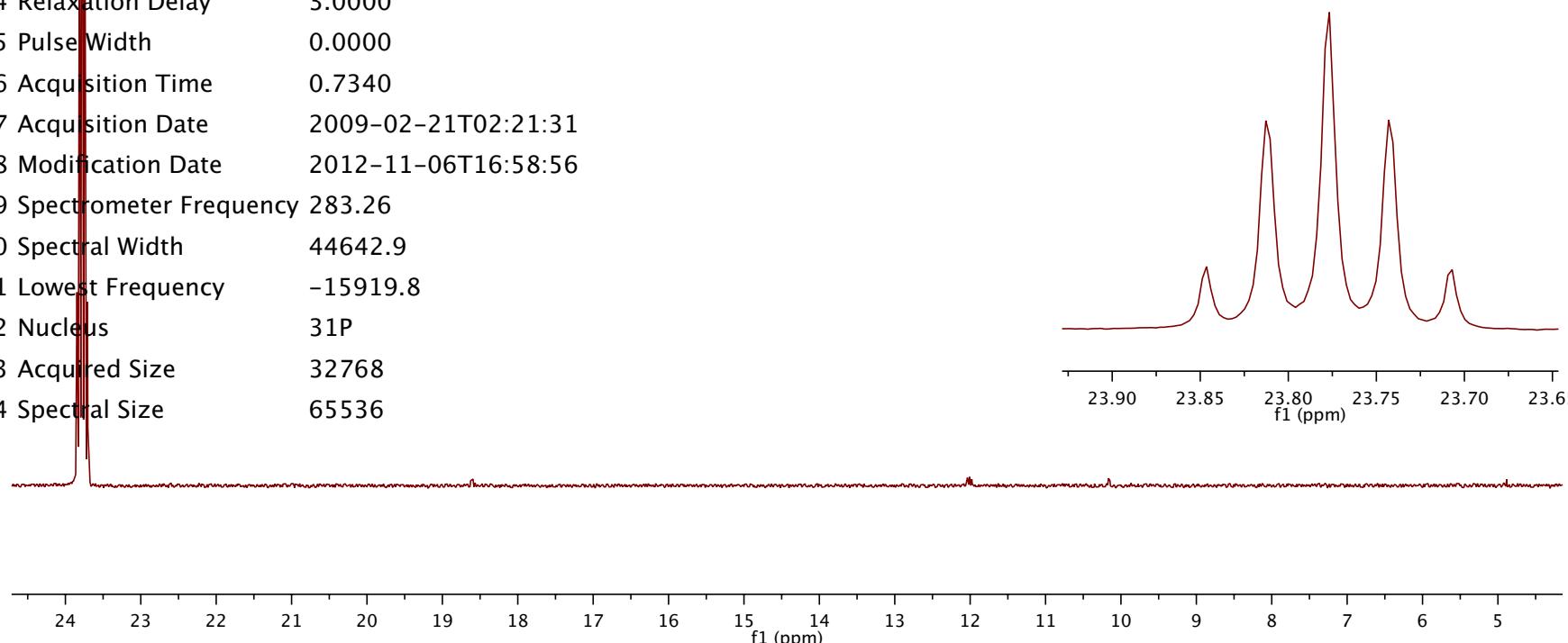
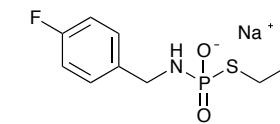
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3 Comment	MT 457
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	cd3od
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	4
13 Receiver Gain	44
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	2.9098
17 Acquisition Date	2009-02-25T01:07:35
18 Modification Date	2012-11-19T11:08:11
19 Spectrometer Frequency	699.74
20 Spectral Width	11261.3
21 Lowest Frequency	-1432.2
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536



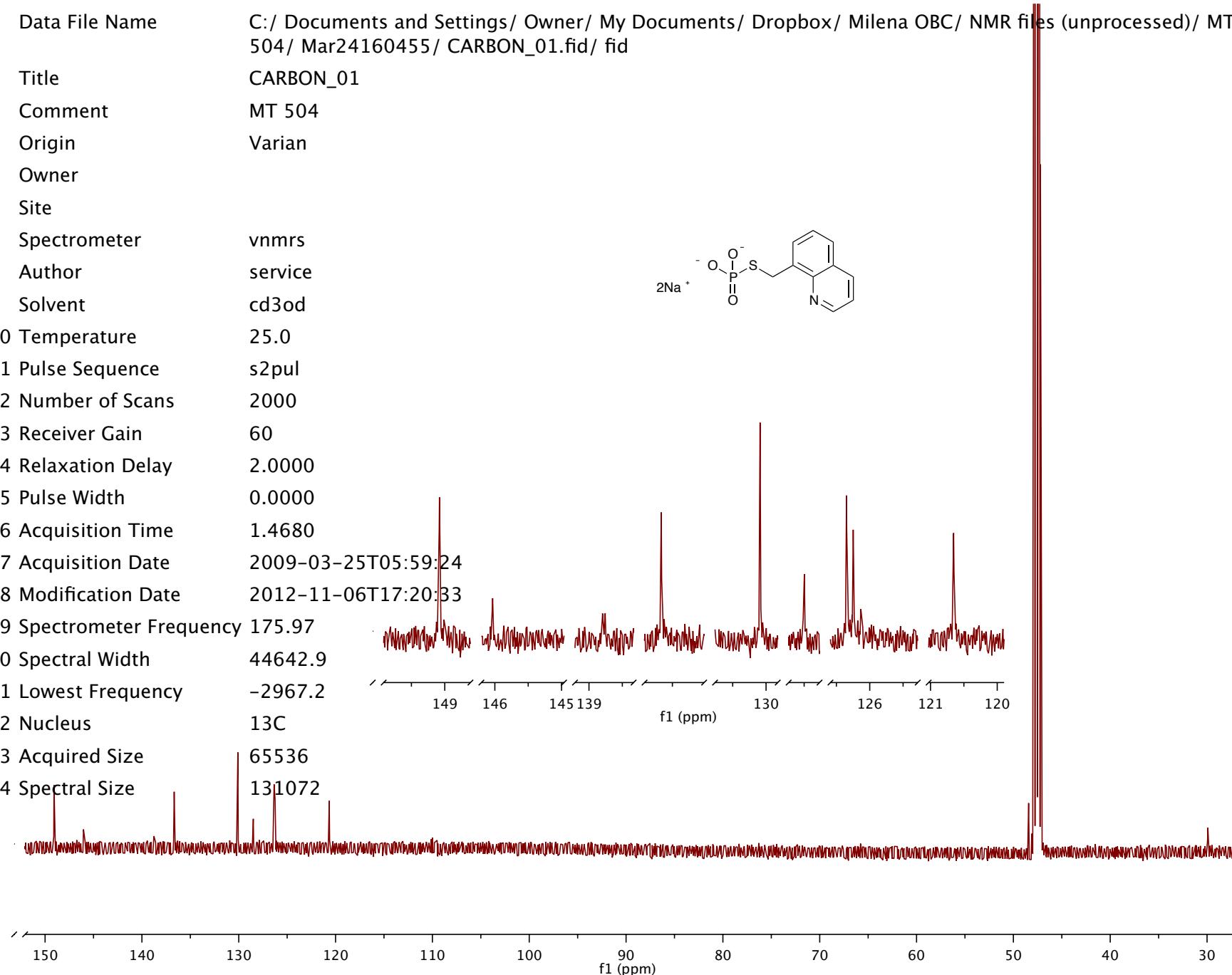
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5	Owner	
6	Site	
7	Spectrometer	vnmrs
8	Author	service
9	Solvent	cd3od
10	Temperature	25.0
11	Pulse Sequence	s2pul
12	Number of Scans	256
13	Receiver Gain	50
14	Relaxation Delay	3.0000
15	Pulse Width	0.0000
16	Acquisition Time	0.7340
17	Acquisition Date	2009-02-21T02:21:31
18	Modification Date	2012-11-06T16:58:56
19	Spectrometer Frequency	283.26
20	Spectral Width	44642.9
21	Lowest Frequency	-15919.8
22	Nucleus	³¹ P
23	Acquired Size	32768
24	Spectral Size	65536

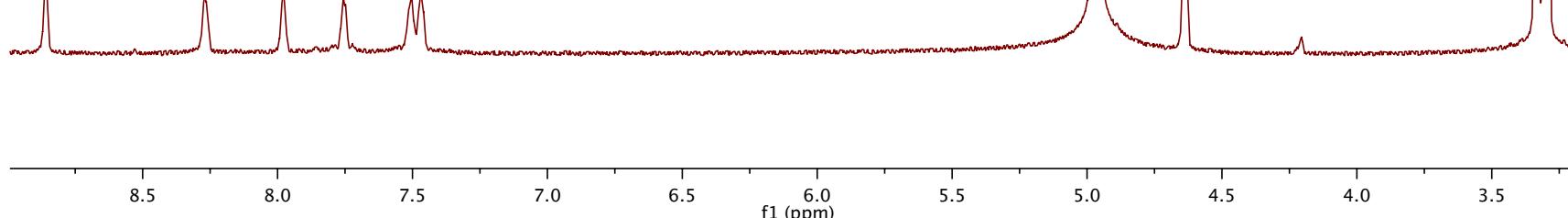
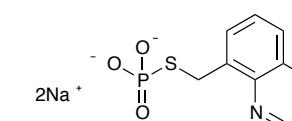
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Parameter	Value
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4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	cd3od
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	2000
13 Receiver Gain	60
14 Relaxation Delay	2.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.4680
17 Acquisition Date	2009-03-25T05:59:24
18 Modification Date	2012-11-06T17:20:33
19 Spectrometer Frequency	175.97
20 Spectral Width	44642.9
21 Lowest Frequency	-2967.2
22 Nucleus	¹³ C
23 Acquired Size	65536
24 Spectral Size	131072



Parameter	Value
1 Data File Name	C:/ Documents and Settings/ Owner/ My Documents/ Dropbox/ Milena OBC/ NMR files (unprocessed)/ MT 504/ Mar23153724/ PROTON_01.fid/ fid
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3 Comment	MT 504
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	cd3od
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	4
13 Receiver Gain	42
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	2.9098
17 Acquisition Date	2009-03-23T16:07:31
18 Modification Date	2012-11-06T17:20:28
19 Spectrometer Frequency	699.74
20 Spectral Width	11261.3
21 Lowest Frequency	-1432.2
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536



Parameter	Value
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3 Comment	MT 504
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	vnmrs
8 Author	service
9 Solvent	cd3od
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	256
13 Receiver Gain	50
14 Relaxation Delay	3.0000
15 Pulse Width	0.0000
16 Acquisition Time	0.7340
17 Acquisition Date	2009-03-19T10:43:33
18 Modification Date	2012-11-06T17:20:26
19 Spectrometer Frequency	283.26
20 Spectral Width	44642.9
21 Lowest Frequency	-15919.8
22 Nucleus	^{31}P
23 Acquired Size	32768
24 Spectral Size	65536

