

## SUPPORTING INFORMATION

№1

# Preparation of a Microsized Cerium Chloride-Based Catalyst and its Application in Michael Addition of $\beta$ -Diketones to Vinyl Ketones

Alexander O. Terent'ev,<sup>a,b</sup> Vera A. Vil',<sup>a</sup> Ivan A. Yaremenko,<sup>a</sup> Oleg V. Bityukov,<sup>a,b</sup>  
Dmitri O. Levitsky,<sup>c</sup> Vladimir V. Chernyshev,<sup>d,e</sup> Gennady I. Nikishin,<sup>a</sup> and Fabrice Fleury.<sup>c</sup>

### AUTHOR ADDRESSES

<sup>a</sup> N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Leninsky prospect 47, Moscow, 119991 Russian Federation.

<sup>b</sup> D. Mendeleev University of Chemical Technology of Russia, Miusskaya square 9, Moscow, 125047 Russian Federation.

<sup>c</sup> UFIP FRE-CNRS 3478, DNA repair team, Université de Nantes, 2 rue de la Houssinière, 44322 Nantes, France.

<sup>d</sup> Department of Chemistry, M.V. Lomonosov Moscow State University, 1-3 Leninskie Gory, Moscow, 119991 Russian Federation.

<sup>e</sup> A. N. Frumkin Institute of Physical Chemistry and Electrochemistry RAS, 31 Leninsky prospect, Moscow, 119071 Russian Federation.

CORRESPONDING AUTHOR E-MAIL ADDRESS [terentev@ioc.ac.ru](mailto:terentev@ioc.ac.ru)

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### <sup>1</sup>H NMR of 6-methylheptane-2,4-dione (**1b**)

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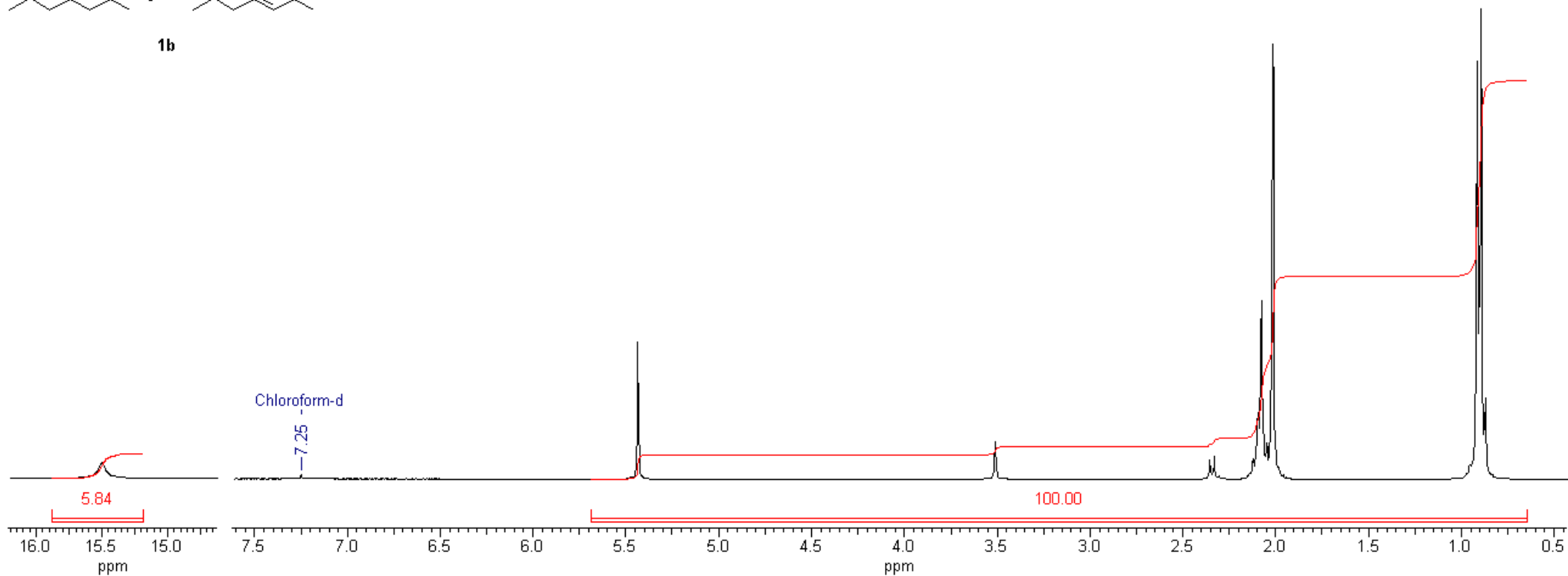
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Frequency (MHz)	300.13
Points Count	8192
Sweep Width (Hz)	6009.62



**1b**



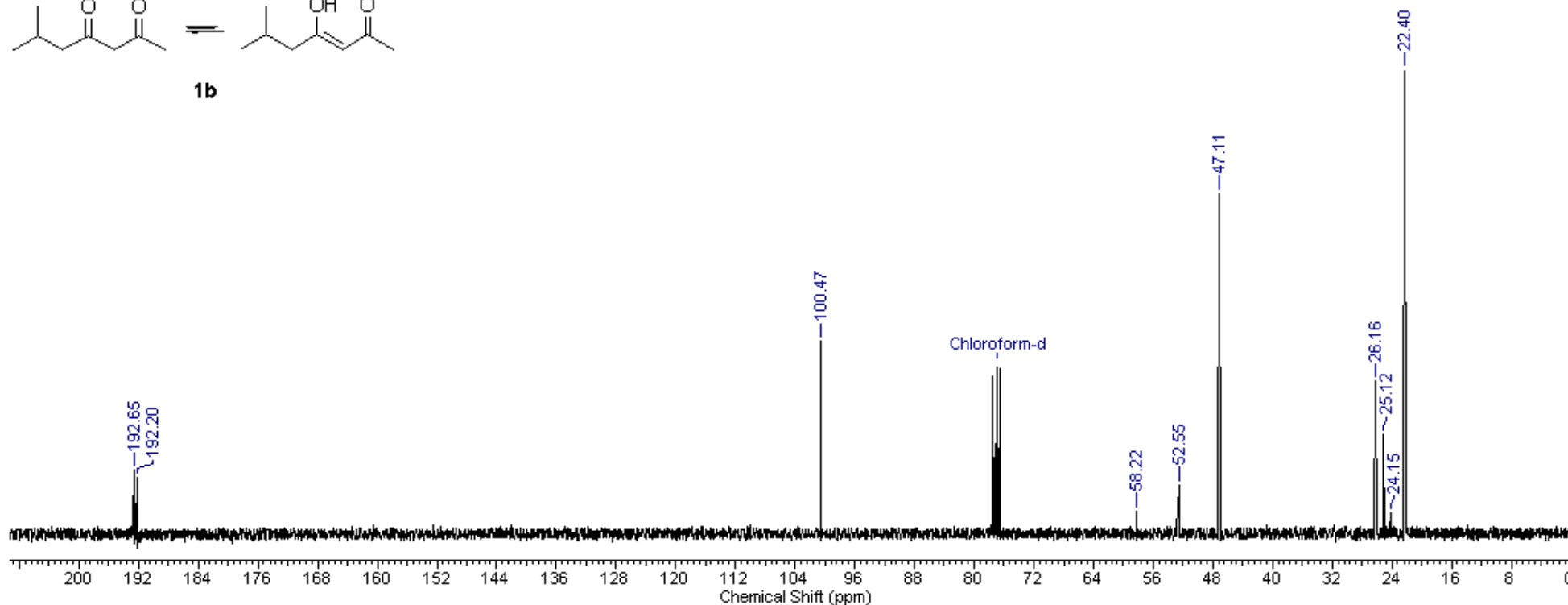
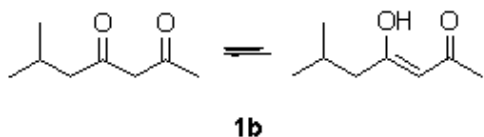
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No.	Annotation	(ppm)
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No.	(ppm)	Value
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2	18 .. 15.1	5.836

<sup>13</sup>C NMR of 6-methylheptane-2,4-dione (**1b**)

<b>Acquisition Time (sec)</b>	0.9006	<b>Date</b>	24 Jul 2013 13:32:48			
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					<b>Frequency (MHz)</b>	75.48
					<b>Points Count</b>	16384
					<b>Temperature (degree C)</b>	26.600



No.	(ppm)	(Hz)	Height
1	22.40	1690.4	1.0000
2	24.15	1823.1	0.0233
3	25.12	1896.1	0.1959
4	26.16	1974.6	0.3141
5	47.11	3555.9	0.7287
6	52.55	3966.1	0.0863
7	58.22	4394.0	0.0280
8	100.47	7583.1	0.4033
9	192.20	14506.4	0.1021
10	192.65	14540.7	0.1185

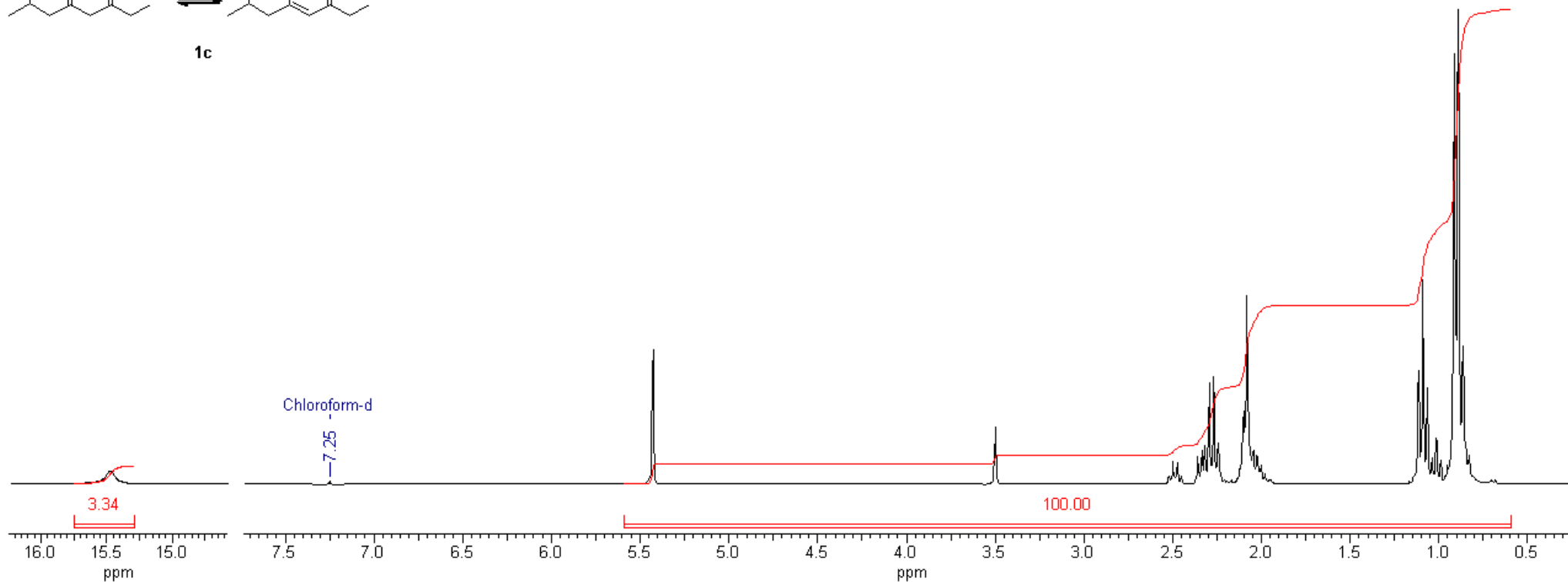
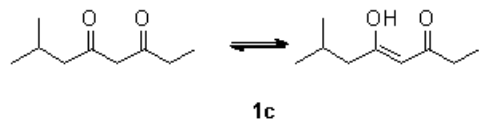
No.	Annotation	(ppm)
1	Chloroform-d	77.00

### <sup>1</sup>H NMR of 7-methyloctane-3,5-dione (**1c**)

Acquisition Time (sec) 0.6759

Date 24 Jul 2013 12:48:00

Nucleus	1H	Number of Transients	1	Original Points Count	8124	Frequency (MHz)	300.13
Pulse Sequence	zg	Solvent	CHLOROFORM-D			Points Count	8192
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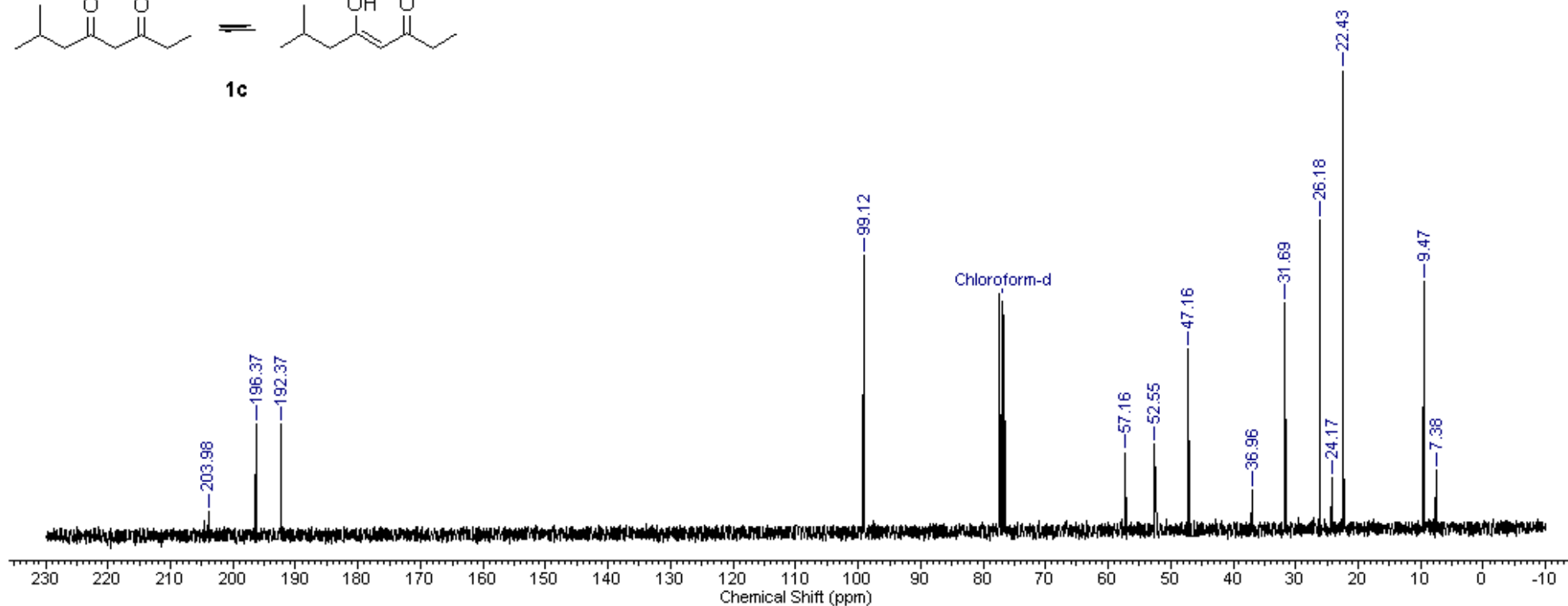
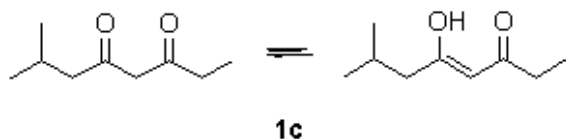
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No.	Annotation	(ppm)
1	Chloroform-d	7.25

No.	(ppm)	Value
1	59 .. 5.5	100.000
2	29 .. 15	3.336

<sup>13</sup>C NMR of 7-methyloctane-3,5-dione (**1c**)

<b>Acquisition Time (sec)</b>	0.9006	<b>Date</b>	24 Jul 2013 12:50:08			
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<b>Pulse Sequence</b>	zgpg30	<b>Solvent</b>	CHLOROFORM-D	<b>Sweep Width (Hz)</b>	18115.94	
					<b>Frequency (MHz)</b>	75.48
					<b>Points Count</b>	16384
					<b>Temperature (degree C)</b>	26.300



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	7.38	557.0	0.1019	8	47.16	3559.2	0.3750
2	9.47	715.1	0.5257	9	52.55	3966.1	0.1604
3	22.43	1692.6	1.0000	10	57.16	4314.4	0.1417
4	24.17	1824.2	0.0832	11	99.12	7481.4	0.5846
5	26.18	1975.7	0.6650	12	192.37	14519.6	0.2043
6	31.69	2391.5	0.4779	13	196.37	14821.5	0.2061
7	36.96	2789.6	0.0574	14	203.98	15395.4	0.0078

No.	Annotation	(ppm)
1	Chloroform-d	77.00



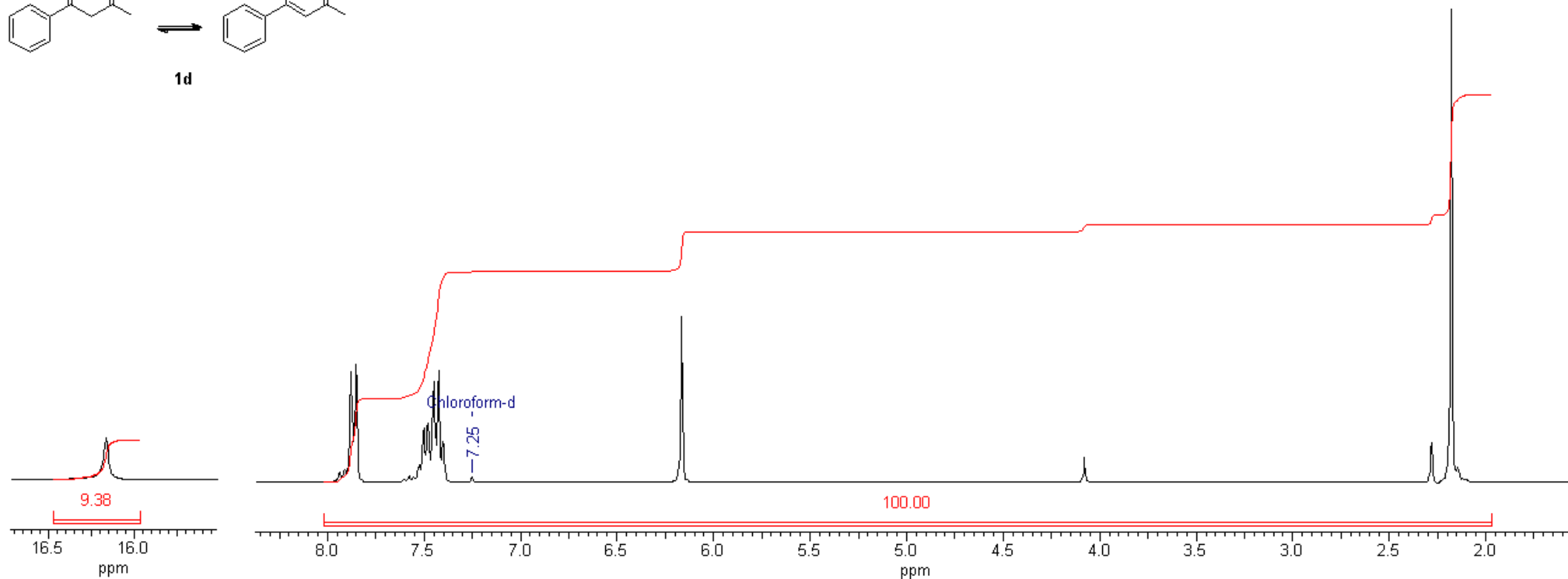
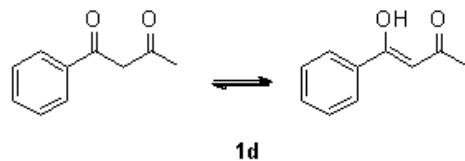
### <sup>1</sup>H NMR of 1-phenylbutane-1,3-dione (**1d**)

Acquisition Time (sec) 0.6759

Date 24 Jul 2013 13:39:12

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Temperature (degree C) 26.600

Frequency (MHz) 300.13  
Points Count 8192  
Sweep Width (Hz) 6009.62



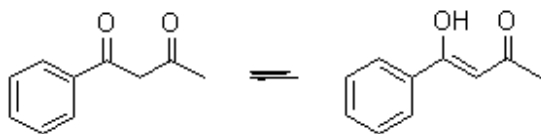
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No.	Annotation	(ppm)
1	Chloroform-d	7.25

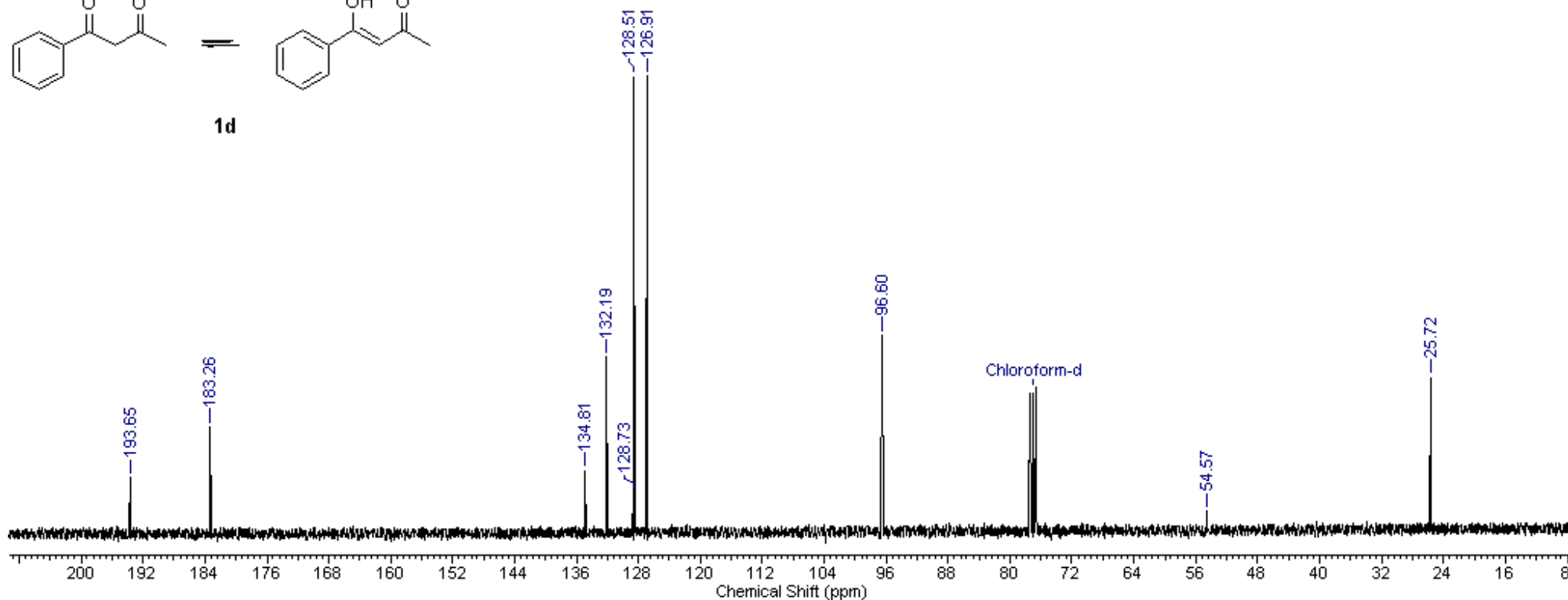
No.	(ppm)	Value
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2	96 .. 16.	9.383

<sup>13</sup>C NMR of 1-phenylbutane-1,3-dione (**1d**)

<b>Acquisition Time (sec)</b>	0.9006	<b>Date</b>	24 Jul 2013 13:39:12			
<b>Nucleus</b>	13C	<b>Number of Transients</b>	170	<b>Original Points Count</b>	16316	
<b>Pulse Sequence</b>	zgpg30	<b>Solvent</b>	CHLOROFORM-D	<b>Sweep Width (Hz)</b>	18115.94	
					<b>Frequency (MHz)</b>	75.48
					<b>Points Count</b>	16384
					<b>Temperature (degree C)</b>	26.500



**1d**



No.	(ppm)	(Hz)	Height
1	25.72	1941.4	0.3209
2	54.57	4118.7	0.0198
3	96.60	7291.2	0.4165
4	126.91	9579.0	1.0000
5	128.51	9699.6	0.9989
6	128.73	9716.2	0.0605
7	132.19	9977.1	0.3670
8	134.81	10175.1	0.1113
9	183.26	13831.9	0.2102
10	193.65	14615.9	0.0957

No.	Annotation	(ppm)
1	Chloroform-d	77.00

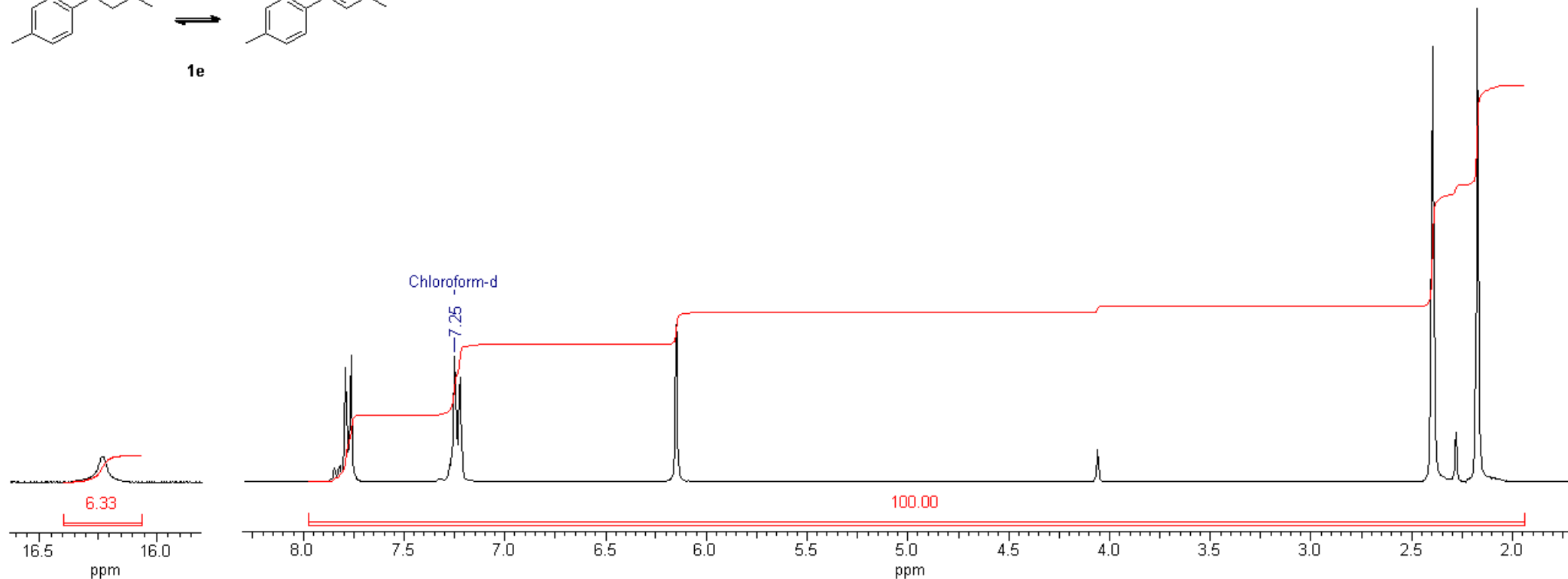
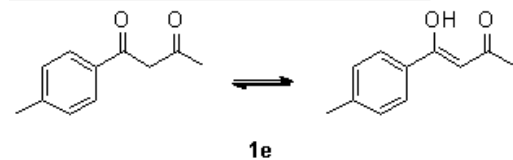
### <sup>1</sup>H NMR of 1-(4-methylphenyl)butane-1,3-dione (**1e**)

Acquisition Time (sec) 0.6759

Date 24 Jul 2013 13:47:44

Nucleus	1H	Number of Transients	1	Original Points Count	8124
Pulse Sequence	zg	Solvent	CHLOROFORM-D	Points Count	8192
Temperature (degree C)	26.600			Sweep Width (Hz)	6009.62

Frequency (MHz)	300.13
Points Count	8192
Sweep Width (Hz)	6009.62



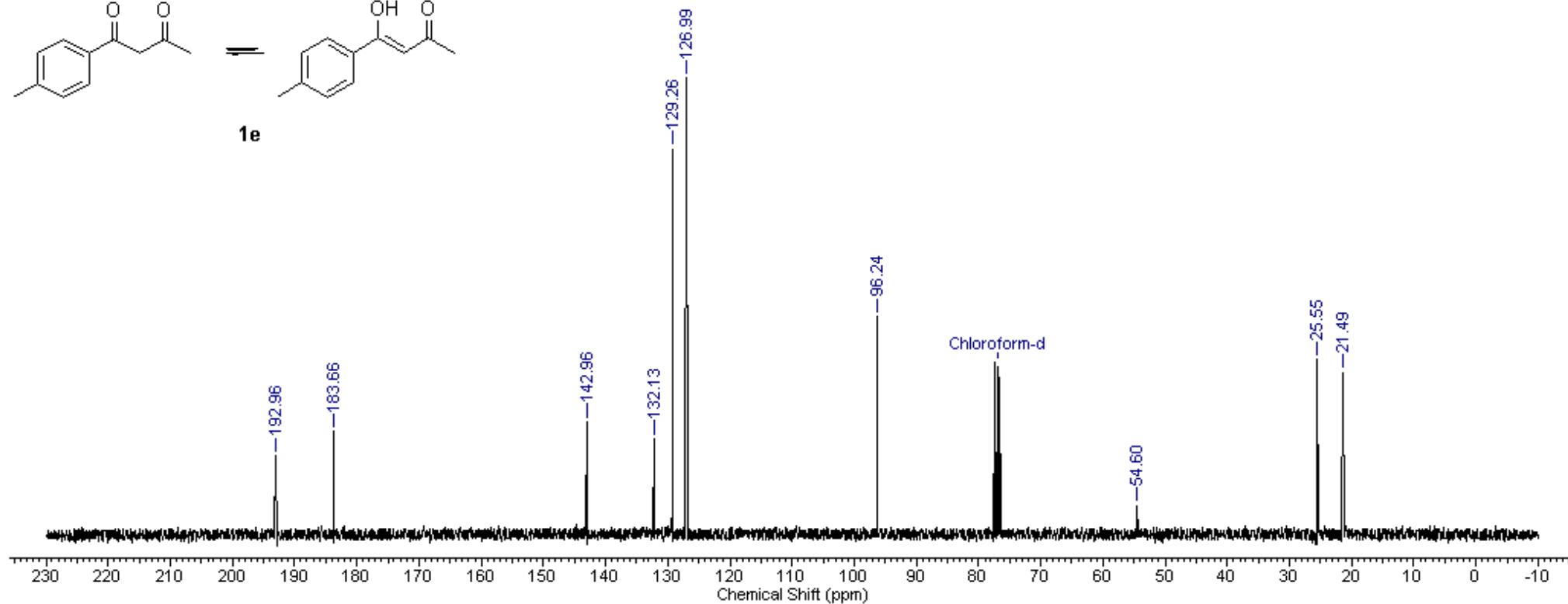
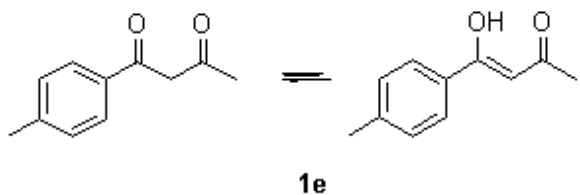
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No.	Annotation	(ppm)
1	Chloroform-d	7.25

No.	(ppm)	Value
1	94 .. 7.9	100.000
2	06 .. 16	6.327

<sup>13</sup>C NMR of 1-(4-methylphenyl)butane-1,3-dione (**1e**)

<b>Acquisition Time (sec)</b>	0.9006	<b>Date</b>	24 Jul 2013 13:47:44		
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<b>Pulse Sequence</b>	zgpg30	<b>Solvent</b>	CHLOROFORM-D	<b>Sweep Width (Hz)</b>	18115.94
				<b>Frequency (MHz)</b>	75.48
				<b>Points Count</b>	16384
				<b>Temperature (degree C)</b>	26.600

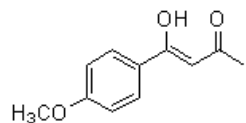


No.	(ppm)	(Hz)	Height
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2	25.55	1928.2	0.3614
3	54.60	4120.9	0.0307
4	96.24	7263.5	0.4595
5	126.99	9584.6	1.0000
6	129.26	9756.0	0.8387
7	132.13	9972.7	0.1831
8	142.96	10789.9	0.2210
9	183.66	13861.7	0.1980
10	192.96	14563.9	0.1436

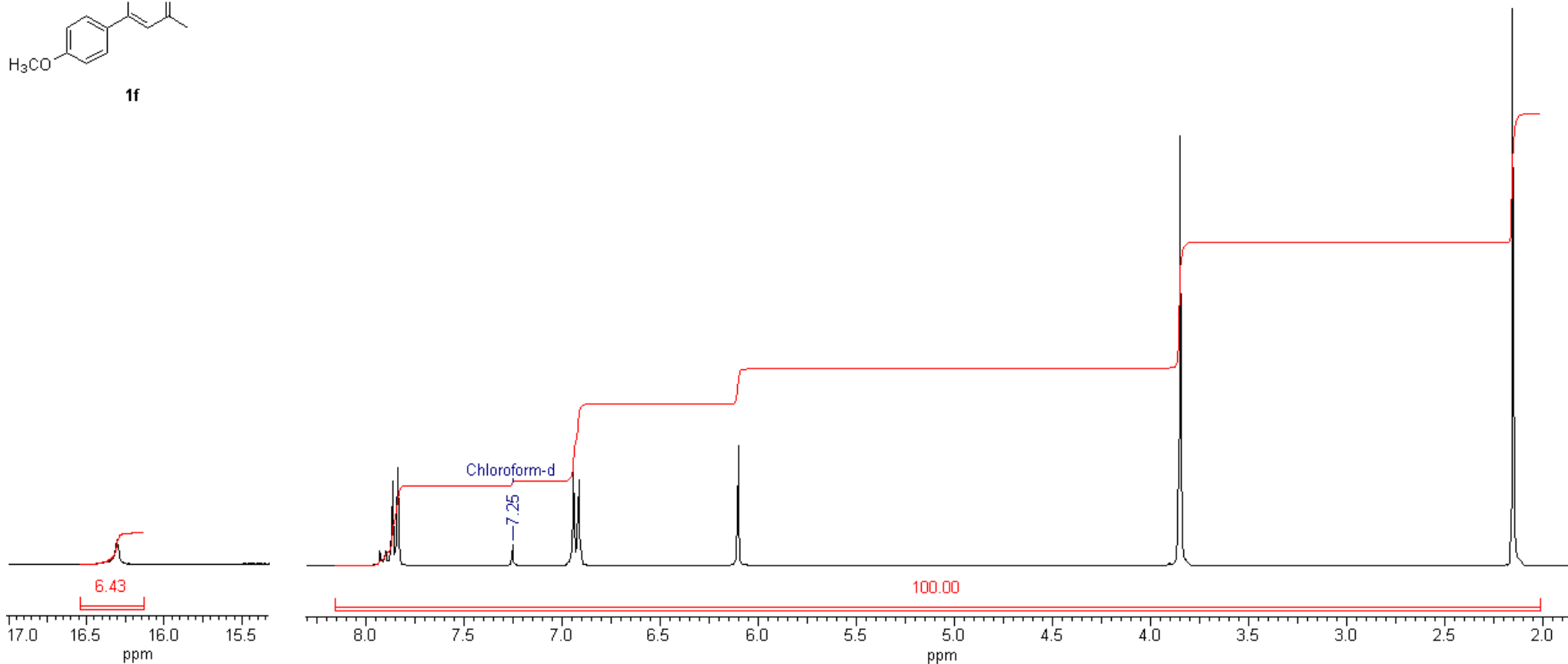
No.	Annotation	(ppm)
1	Chloroform-d	77.00

<sup>1</sup>H NMR of 1-(4-methoxyphenyl)butane-1,3-dione (**1f**)

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<b>Temperature (degree C)</b> 21.900				



**1f**



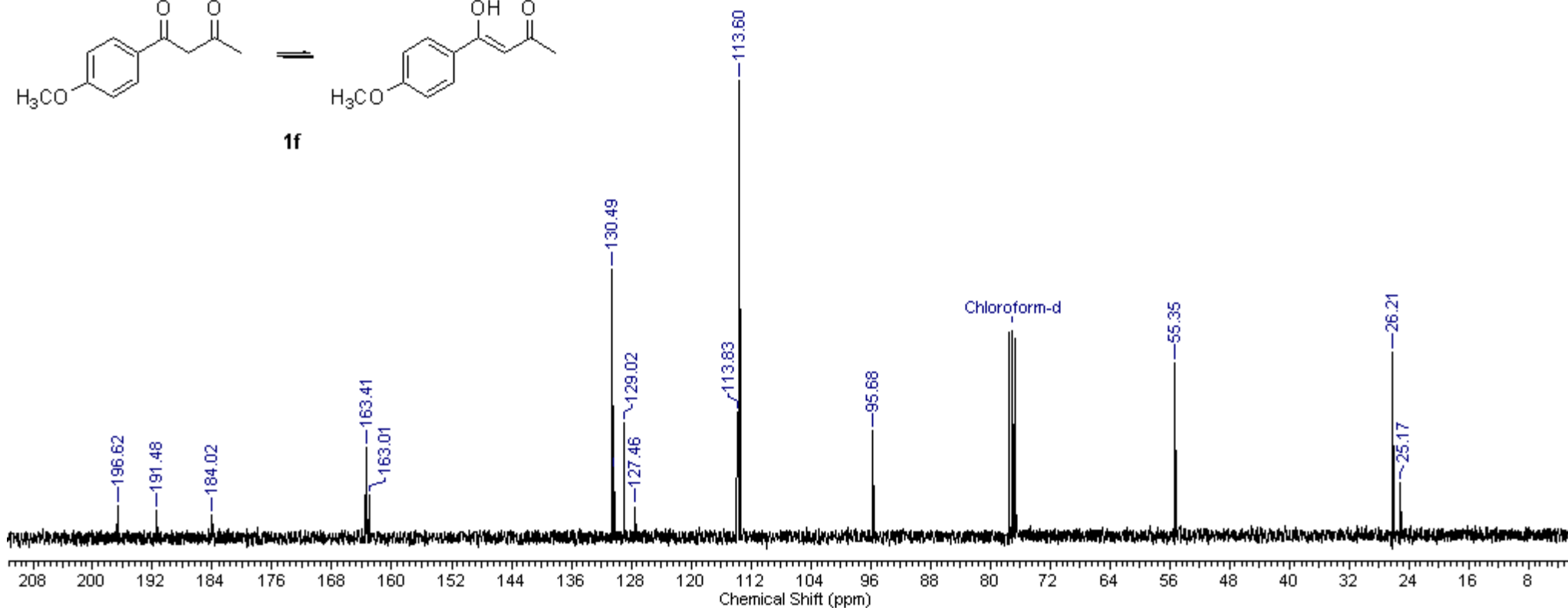
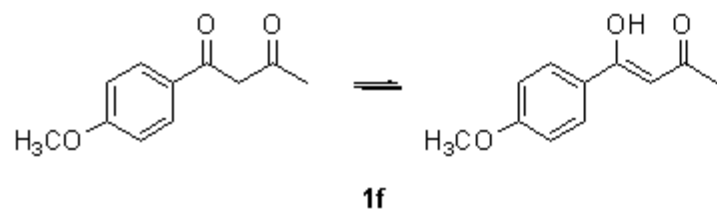
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1	7.25	2175.8	0.0373

No.	Annotation	(ppm)
1	Chloroform-d	7.25

No.	(ppm)	Value
1	.02 .. 8.1	100.000
2	.13 .. 16.1	6.426

<sup>13</sup>C NMR of 1-(4-methoxyphenyl)butane-1,3-dione (**1f**)

<b>Acquisition Time (sec)</b>	0.9006	<b>Date</b>	24 Jul 2013 13:58:24	
<b>Nucleus</b>	13C	<b>Number of Transients</b>	248	<b>Original Points Count</b>
<b>Pulse Sequence</b>	zgpg30	<b>Solvent</b>	CHLOROFORM-D	<b>Sweep Width (Hz)</b>
				<b>Frequency (MHz)</b>
				<b>Points Count</b>
				<b>Temperature (degree C)</b>



No.	(ppm)	(Hz)	Height
1	25.17	1899.4	0.0815
2	26.21	1977.9	0.3805
3	55.35	4177.3	0.3556
4	95.68	7221.5	0.2003
5	113.60	8573.9	1.0000
6	113.83	8591.6	0.2435
7	127.46	9619.9	0.0278
8	129.02	9738.3	0.2197

No.	(ppm)	(Hz)	Height
9	130.27	9832.3	0.1095
10	130.49	9848.8	0.5697
11	163.01	12303.7	0.0537
12	163.41	12333.5	0.1621
13	184.02	13889.4	0.0082
14	191.48	14452.2	0.0178
15	196.62	14840.3	0.0295

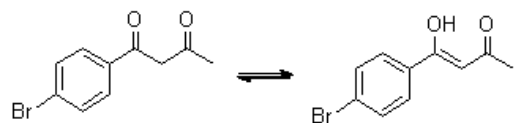
No.	Annotation	(ppm)
1	Chloroform-d	77.00

### <sup>1</sup>H NMR of 1-(4-bromophenyl)butane-1,3-dione (**1g**)

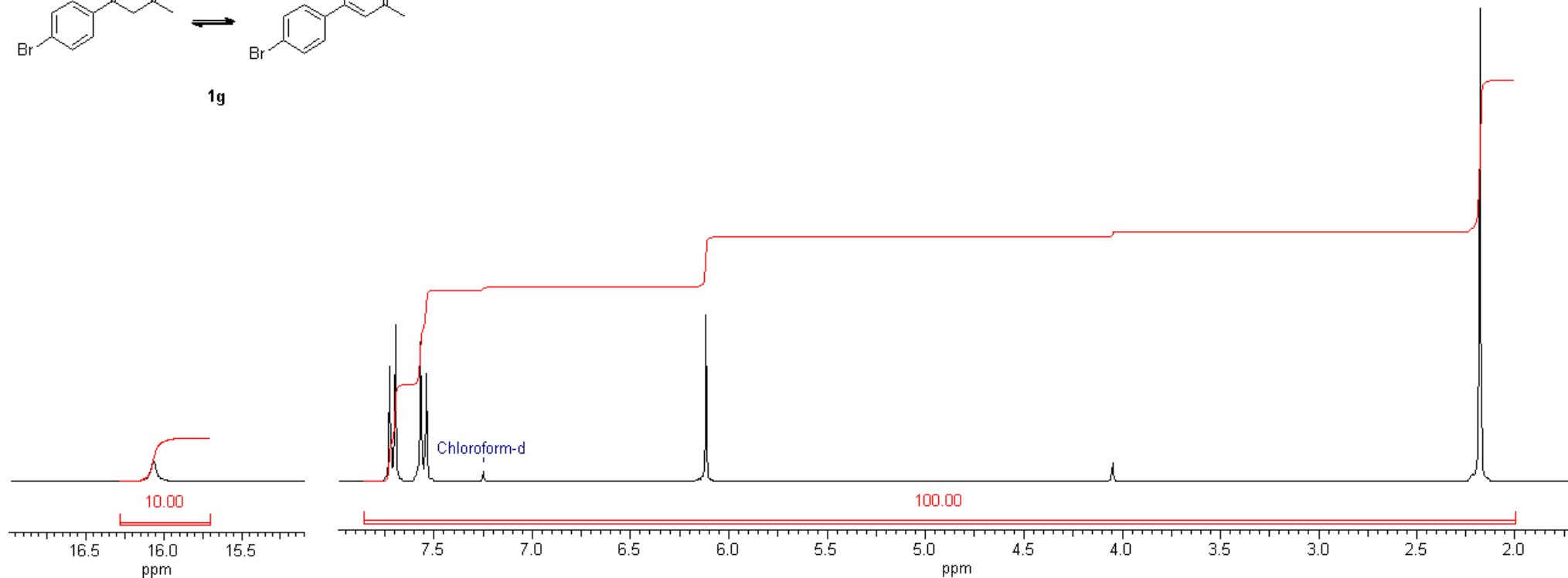
Acquisition Time (sec) 0.6759

Date 11 Sep 2013 11:09:52

Nucleus	1H	Number of Transients	1	Original Points Count	8124	Frequency (MHz)	300.13
Pulse Sequence	zg	Solvent	CHLOROFORM-D	Points Count	8192	Sweep Width (Hz)	6009.62
Temperature (degree C)	23.900						



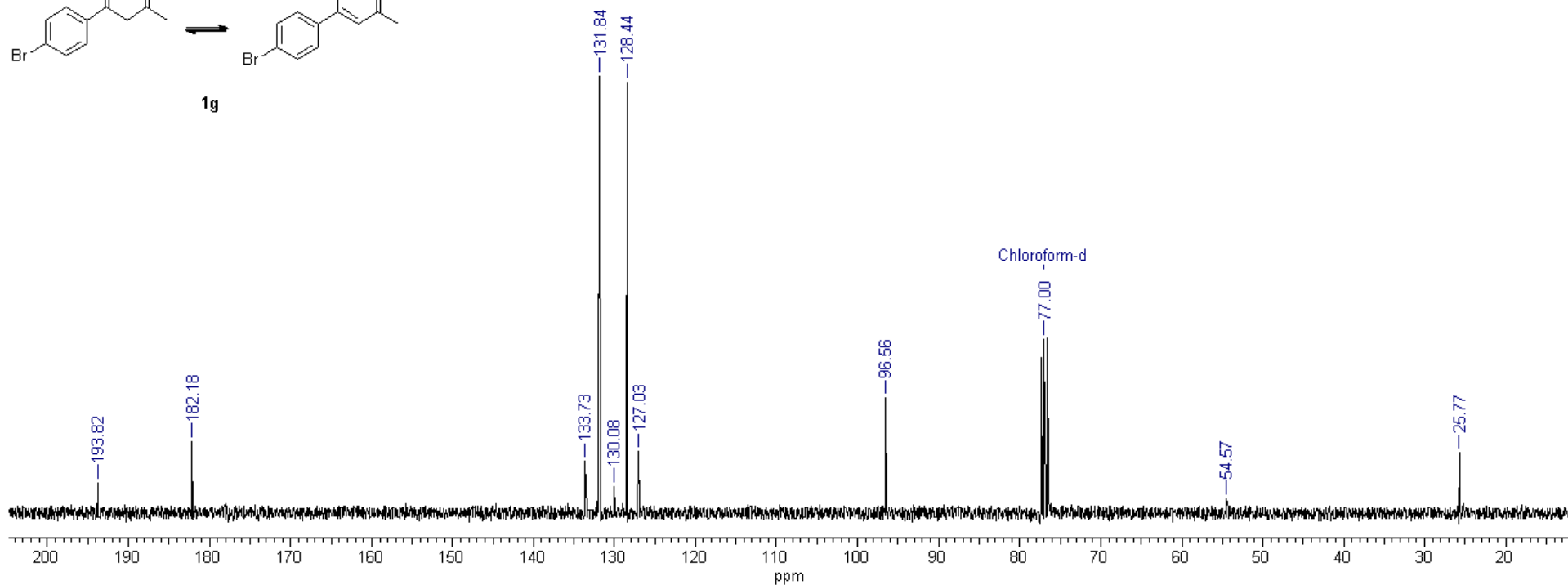
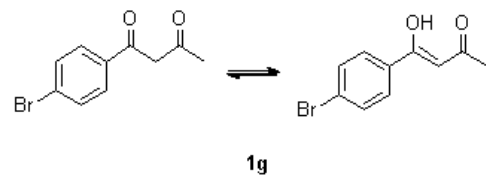
**1g**



No.	Annotation	(ppm)	No.	(ppm)	Value
1	Chloroform-d	7.25	1	.00 .. 7.8	100.000

<sup>13</sup>C NMR of 1-(4-bromophenyl)butane-1,3-dione (**1g**)

<b>Acquisition Time (sec)</b> 0.4503		<b>Date</b> 11 Sep 2013 13:28:32		<b>Frequency (MHz)</b> 75.48	
<b>Nucleus</b> <sup>13</sup> C	<b>Number of Transients</b> 148	<b>Original Points Count</b> 16316	<b>Points Count</b> 16384		
<b>Pulse Sequence</b> zgpg30	<b>Solvent</b> CHLOROFORM-D		<b>Sweep Width (Hz)</b> 18115.94		
<b>Temperature (degree C)</b> 23.600					



No.	(ppm)	(Hz)	Height
1	25.77	1944.7	0.1632
2	54.57	4118.7	0.0624
3	77.00	5811.6	0.4165
4	96.56	7287.8	0.2851
5	127.03	9587.9	0.1669
6	128.44	9694.0	0.9860
7	130.08	9817.9	0.0881
8	131.84	9950.6	1.0000
9	133.73	10093.2	0.1452
10	182.18	13750.0	0.1893
11	193.82	14629.1	0.0971

No.	Annotation	(ppm)
1	Chloroform-d	77.00

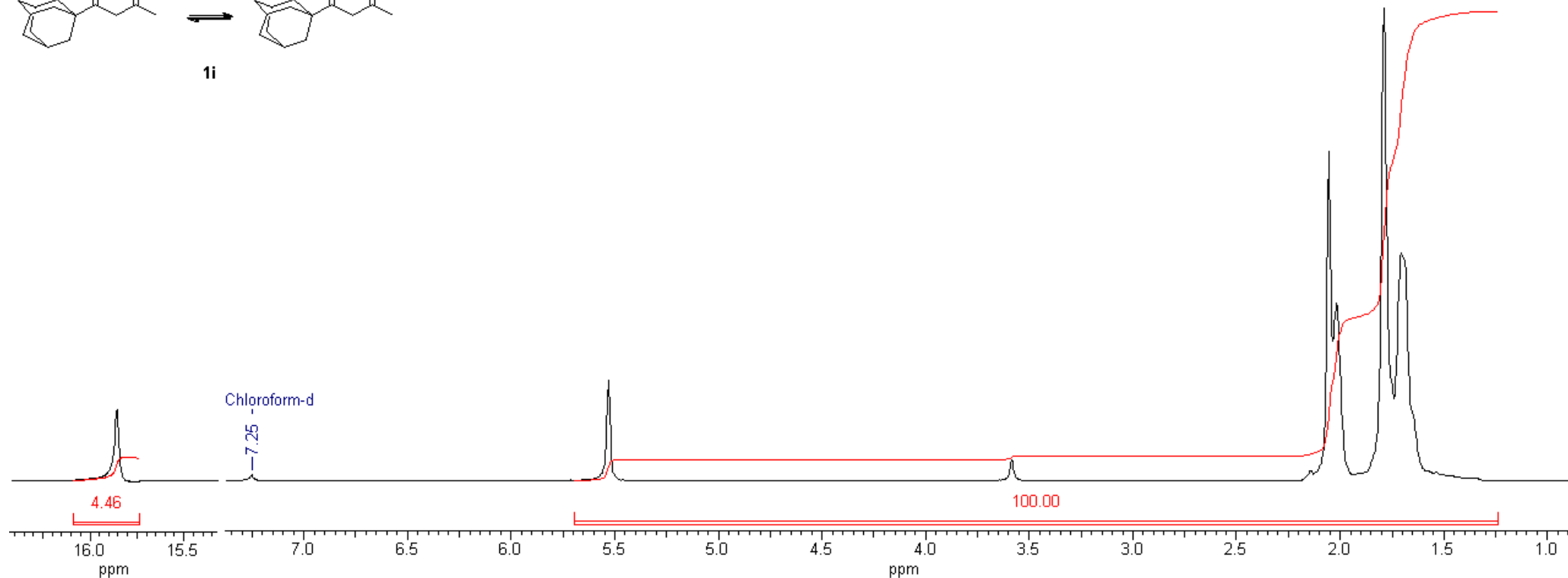
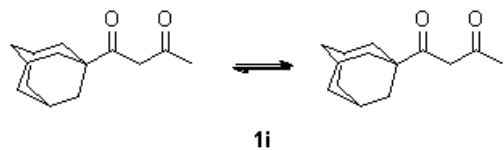


### <sup>1</sup>H NMR of 1-(1-adamantyl)butane-1,3-dione (**1i**)

Acquisition Time (sec) 0.6759

Date 24 Jul 2013 13:20:00

Nucleus	1H	Number of Transients	1	Original Points Count	8124	Frequency (MHz)	300.13
Pulse Sequence	zg	Solvent	CHLOROFORM-D			Points Count	8192
Temperature (degree C)	26.400					Sweep Width (Hz)	6009.62



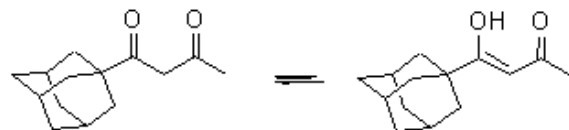
No.	(ppm)	(Hz)	Height
1	7.25	2176.0	0.0119

No.	Annotation	(ppm)
1	Chloroform-d	7.25

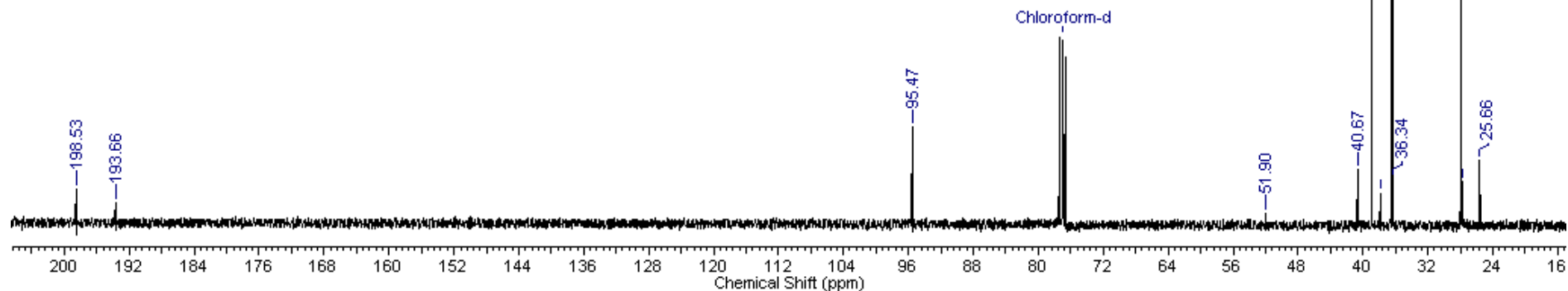
No.	(ppm)	Value
1	.24 .. 5.6	100.000
2	.76 .. 16.	4.438

<sup>13</sup>C NMR of 1-(1-adamantyl)butane-1,3-dione (**1i**)

<b>Acquisition Time (sec)</b>	0.9006	<b>Date</b>	24 Jul 2013 13:20:00		
<b>Nucleus</b>	13C	<b>Number of Transients</b>	273	<b>Original Points Count</b>	16316
<b>Pulse Sequence</b>	zgpg30	<b>Solvent</b>	CHLOROFORM-D	<b>Sweep Width (Hz)</b>	18115.94
				<b>Frequency (MHz)</b>	75.48
				<b>Points Count</b>	16384
				<b>Temperature (degree C)</b>	26.400



**1i**



No.	(ppm)	(Hz)	Height
1	25.66	1937.0	0.1233
2	27.74	2094.0	0.0771
3	27.99	2112.8	0.6325
4	36.34	2743.1	0.0832
5	36.53	2757.5	1.0000
6	37.77	2850.4	0.0521
7	38.92	2937.7	0.8746
8	40.67	3069.3	0.1028
9	51.90	3917.5	0.0068
10	95.47	7206.0	0.1963
11	193.66	14617.0	0.0309
12	198.53	14984.1	0.0612

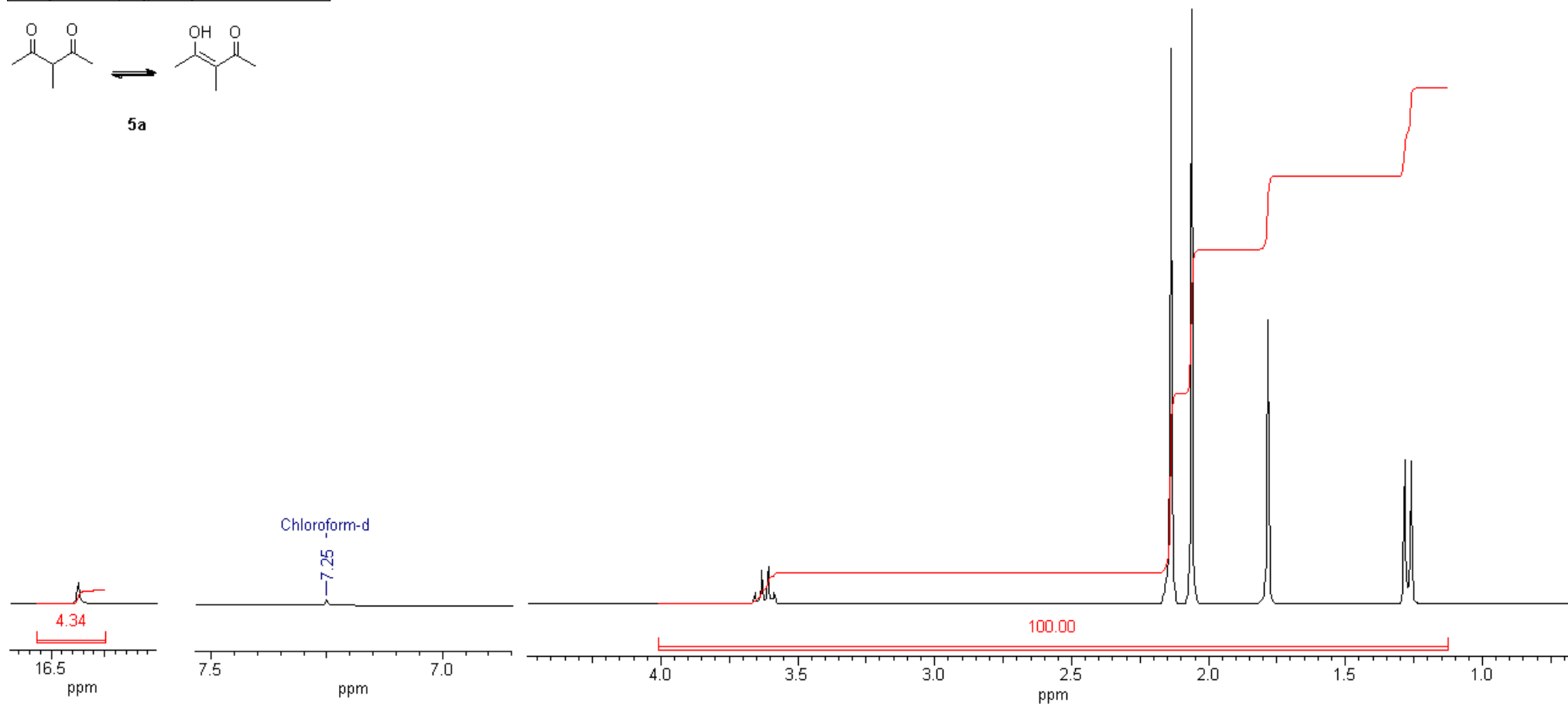
No.	Annotation	(ppm)
1	Chloroform-d	77.00

<sup>1</sup>H NMR of 3-methylpentane-2,4-dione (**5a**)

<b>Acquisition Time (sec)</b>	0.5416	<b>Comment</b>	Avance-300, 1H CDCl3	<b>Date</b>	14 Sep 2013 09:10:24
<b>Nucleus</b>	1H	<b>Number of Transients</b>	1	<b>Original Points Count</b>	8124
<b>Pulse Sequence</b>	zg	<b>Solvent</b>	CHLOROFORM-D	<b>Points Count</b>	8192
<b>Temperature (degree C)</b>	23.300			<b>Sweep Width (Hz)</b>	7500.00



**5a**



No.	(ppm)	(Hz)	Height
1	7.25	2175.8	0.0177

No.	Annotation	(ppm)
1	Chloroform-d	7.25

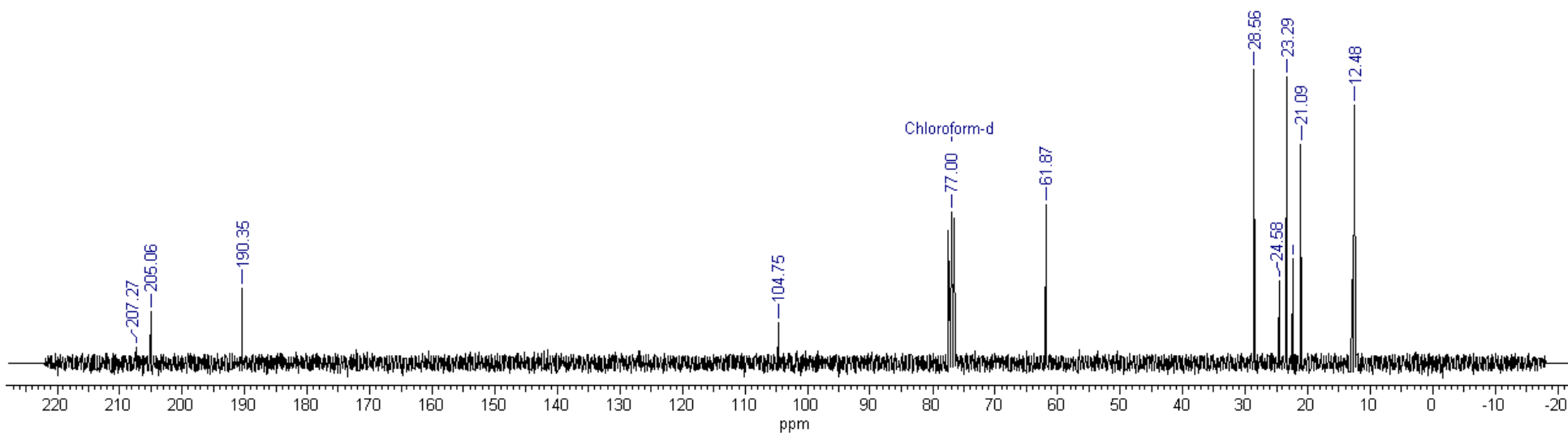
No.	(ppm)	Value
1	12 .. 4.0	100.000
2	25 .. 16.4	4.337

<sup>13</sup>C NMR of 3-methylpentane-2,4-dione (**5a**)

<b>Acquisition Time (sec)</b> 0.4501			<b>Date</b> 14 Sep 2013 09:25:20		
<b>Nucleus</b> <sup>13</sup> C			<b>Frequency (MHz)</b> 75.48		
<b>Pulse Sequence</b> zgpgg baseopt			<b>Points Count</b> 16384		
<b>Temperature (degree C)</b> 23.900			<b>Sweep Width (Hz)</b> 18115.94		
<b>Number of Transients</b> 216			<b>Original Points Count</b> 16308		
<b>Solvent</b> CHLOROFORM-D					



**5a**

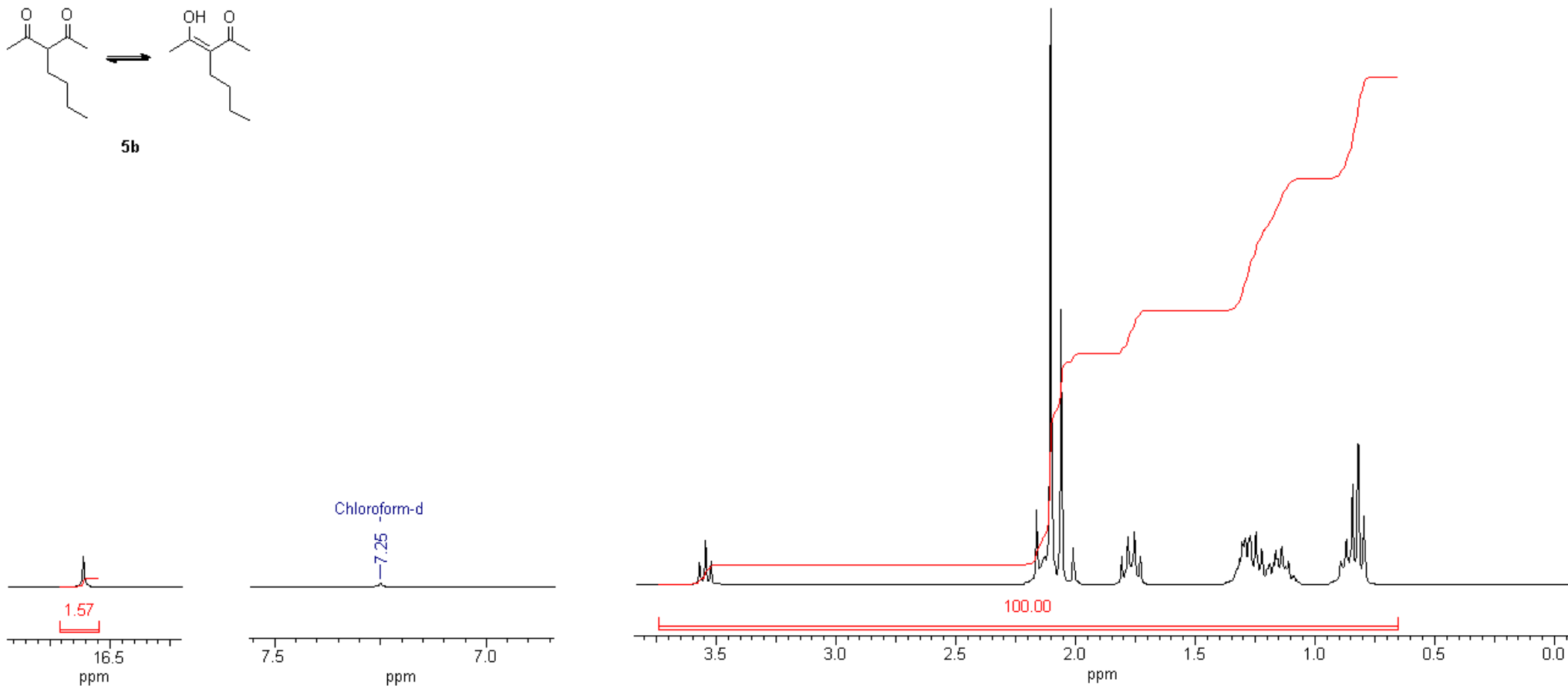
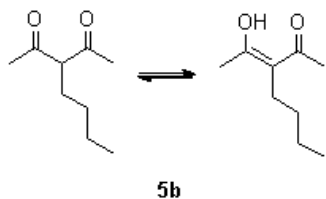


No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	12.48	941.8	0.8788	7	61.87	4669.3	0.5389
2	21.09	1592.0	0.7466	8	77.00	5811.6	0.5140
3	22.43	1692.6	0.3551	9	104.75	7905.9	0.1377
4	23.29	1757.8	0.9736	10	190.35	14367.0	0.2554
5	24.58	1855.1	0.2810	11	205.06	15477.2	0.1734
6	28.56	2155.9	1.0000	12	207.27	15644.2	0.0520

No.	Annotation	(ppm)
1	Chloroform-d	77.00

### <sup>1</sup>H NMR of 3-butylpentane-2,4-dione (**5b**)

<b>Acquisition Time (sec)</b>	0.5416	<b>Comment</b>	Avance-300, 1H CDCl3	<b>Date</b>	14 Sep 2013 08:59:44
<b>Nucleus</b>	1H	<b>Number of Transients</b>	1	<b>Original Points Count</b>	8124
<b>Pulse Sequence</b>	zg	<b>Solvent</b>	CHLOROFORM-D	<b>Points Count</b>	8192
<b>Temperature (degree C)</b>	23.300			<b>Sweep Width (Hz)</b>	7500.00



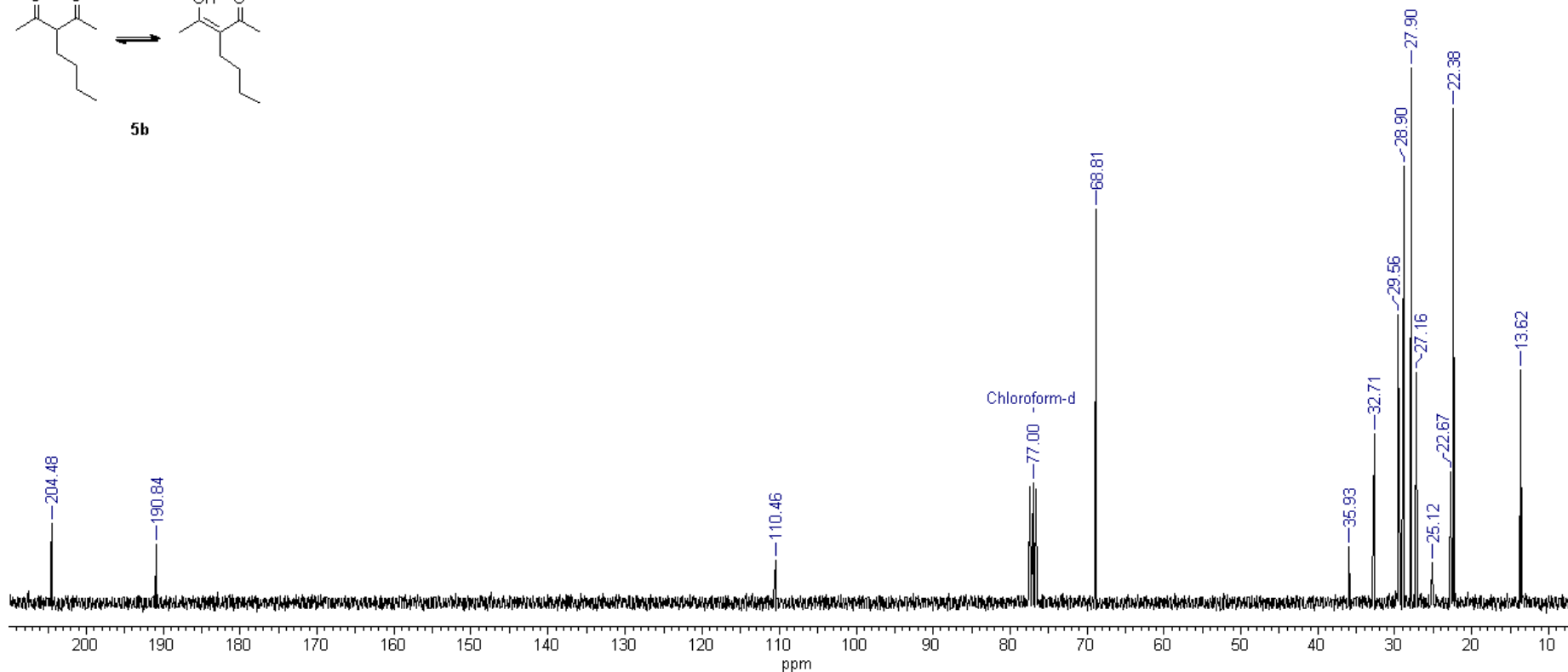
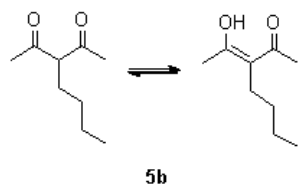
No.	(ppm)	(Hz)	Height
1	7.25	2175.8	0.0062

No.	Annotation	(ppm)
1	Chloroform-d	7.25

No.	(ppm)	Value
1	85 .. 3.7	100.000
2	54 .. 16.	1.574

<sup>13</sup>C NMR of 3-butylpentane-2,4-dione (**5b**)

Acquisition Time (sec)	0.4501	Date	14 Sep 2013 09:36:00
Nucleus	13C	Number of Transients	172
Pulse Sequence	zgpg baseopt	Original Points Count	16308
Temperature (degree C)	23.900	Solvent	CHLOROFORM-D
		Points Count	16384
		Sweep Width (Hz)	18115.94



No.	(ppm)	(Hz)	Height
1	13.62	1028.0	0.4361
2	13.72	1035.7	0.2006
3	22.38	1889.2	0.9237
4	22.51	1899.2	0.3446
5	22.67	1711.4	0.2457
6	25.12	1896.0	0.0752
7	27.16	2049.7	0.4320
8	27.90	2106.1	1.0000
9	28.90	2181.3	0.8161

No.	(ppm)	(Hz)	Height
10	29.56	2231.1	0.5393
11	32.71	2468.8	0.3177
12	35.93	2712.1	0.1047
13	68.81	5193.4	0.7360
14	77.00	5811.6	0.2251
15	110.46	8337.2	0.0788
16	190.84	14403.5	0.1102
17	204.48	15432.9	0.1484

No.	Annotation	(ppm)
1	Chloroform-d	77.00

### <sup>1</sup>H NMR of 3-hexylpentane-2,4-dione (**5c**)

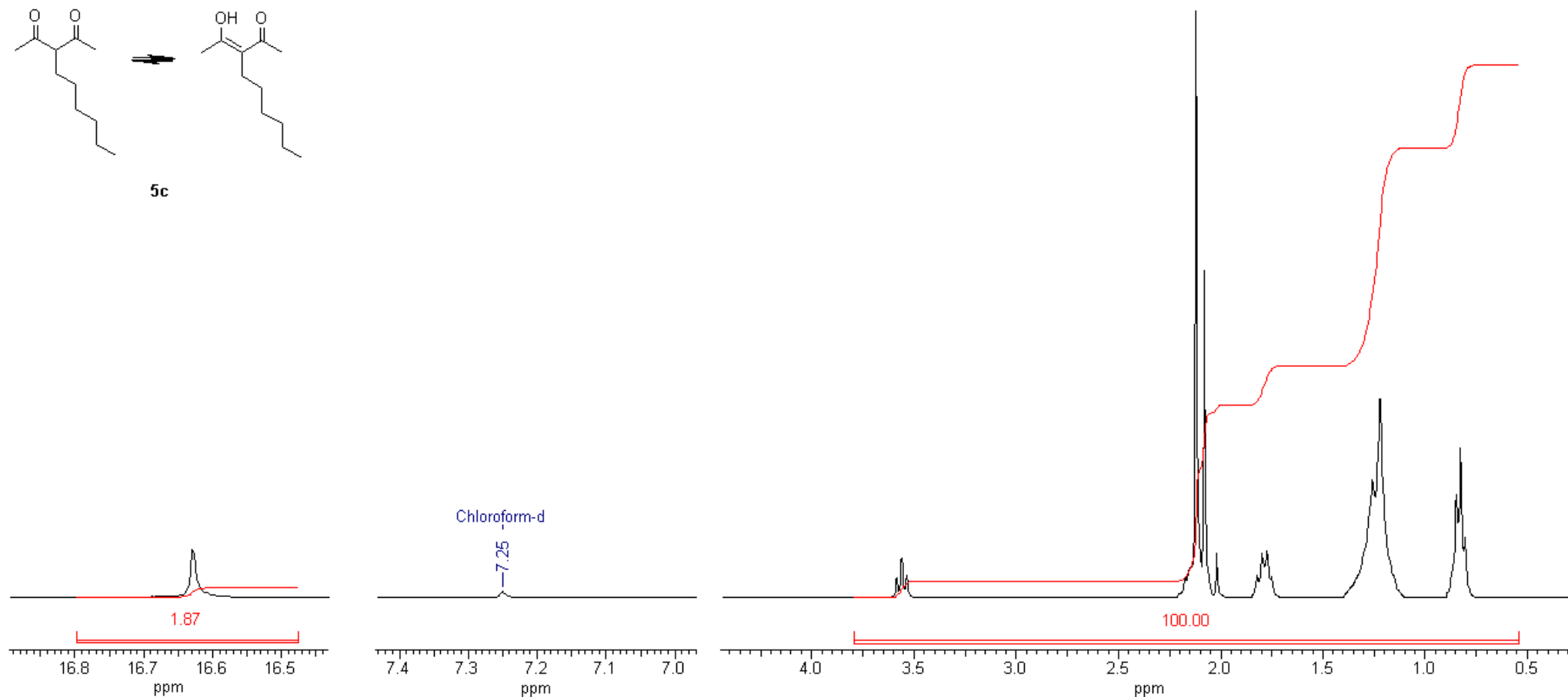
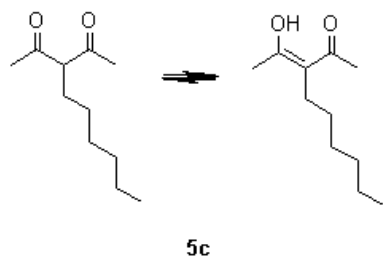
Acquisition Time (sec) 0.6759

Date 01 Aug 2013 12:56:32

Nucleus 1H  
 Pulse Sequence zg  
 Temperature (degree C) 26.400

Number of Transients 1  
 Solvent CHLOROFORM-D  
 Original Points Count 8124

Frequency (MHz) 300.13  
 Points Count 8192  
 Sweep Width (Hz) 6009.62



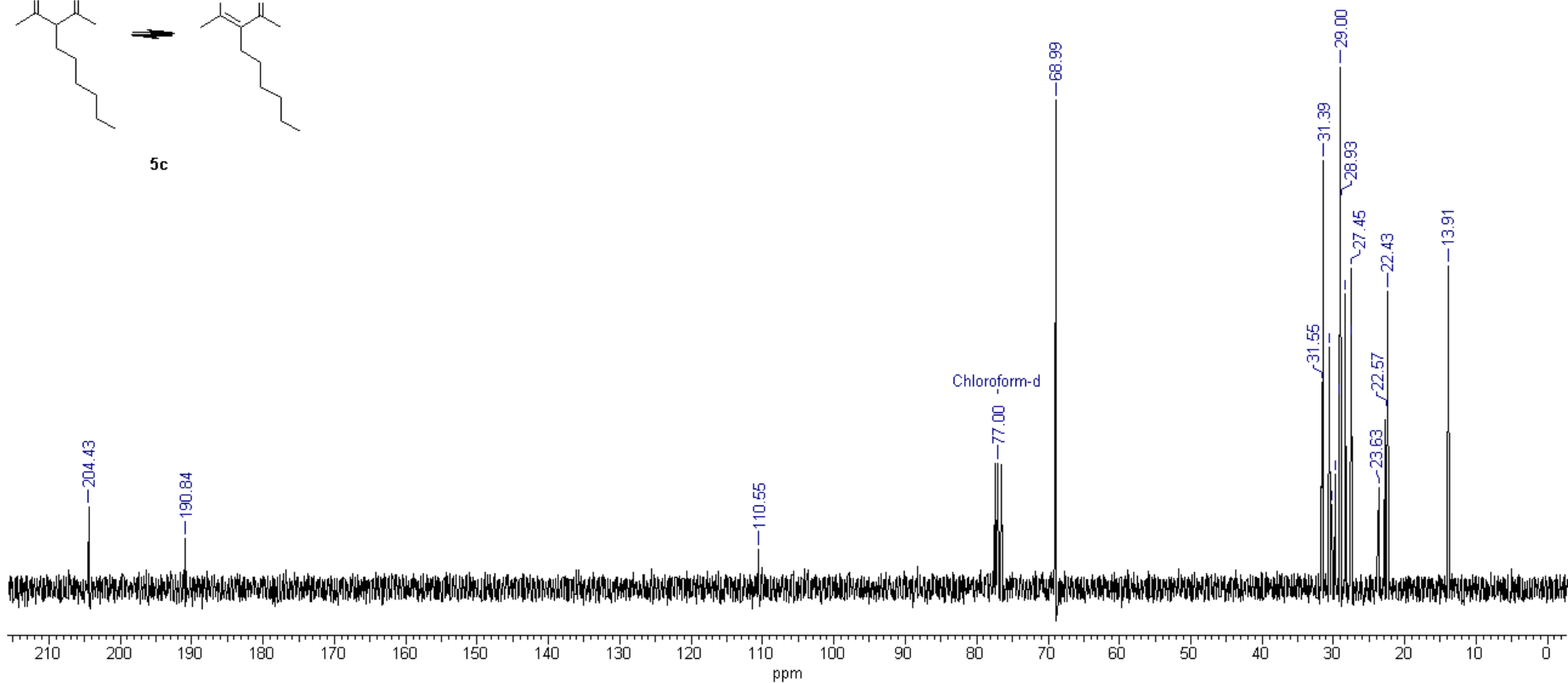
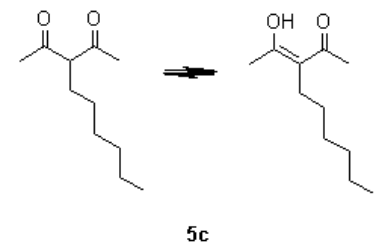
No.	(ppm)	(Hz)	Height
1	7.25	2176.0	0.0112

No.	Annotation	(ppm)
1	Chloroform-d	7.25

No.	(ppm)	Value
1	.54 .. 3.7	100.000
2	.48 .. 16.6	1.866

<sup>13</sup>C NMR of 3-hexylpentane-2,4-dione (**5c**)

<b>Acquisition Time (sec)</b> 0.4501				<b>Date</b> 30 Aug 2013 09:44:32	
<b>Nucleus</b> 13C		<b>Number of Transients</b> 181		<b>Frequency (MHz)</b> 75.48	
<b>Pulse Sequence</b> zgpg baseopt		<b>Solvent</b> CHLOROFORM-D		<b>Points Count</b> 16384	
		<b>Original Points Count</b> 16308		<b>Sweep Width (Hz)</b> 18115.94	
				<b>Temperature (degree C)</b> 26.200	



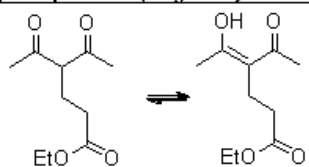
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	13.91	1050.1	0.6186	8	28.27	2133.8	0.5653	15	31.39	2369.3	0.8206
2	22.43	1692.6	0.5718	9	28.93	2183.5	0.7472	16	31.55	2381.5	0.3959
3	22.57	1703.6	0.3425	10	29.00	2189.1	1.0000	17	68.99	5206.7	0.9370
4	22.75	1716.9	0.3251	11	29.21	2204.5	0.3669	18	77.00	5811.6	0.2399
5	23.63	1783.2	0.1927	12	29.71	2242.1	0.2200	19	110.55	8343.8	0.0756
6	27.45	2071.8	0.6155	13	30.29	2286.4	0.1600	20	190.84	14403.5	0.0949
7	27.54	2078.5	0.4804	14	30.59	2308.5	0.4629	21	204.43	15429.6	0.1550

No.	Annotation	(ppm)
1	Chloroform-d	77.00

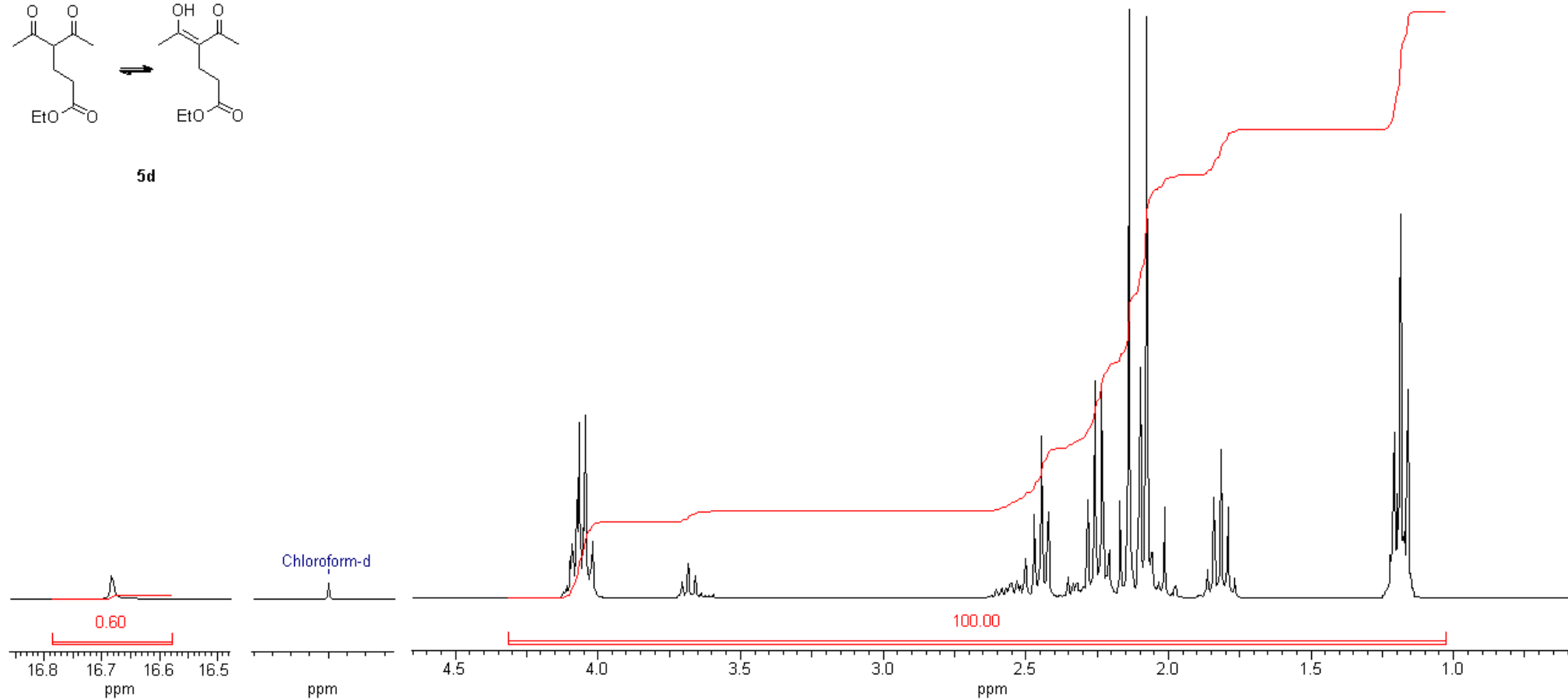


<sup>1</sup>H NMR of ethyl 4-acetyl-5-oxohexanoate (**5d**)

<b>Acquisition Time (sec)</b>	0.5416	<b>Comment</b>	Avance-300, 1H CDCl3		<b>Date</b>	21 Sep 2013 08:42:40		
<b>Nucleus</b>	1H	<b>Number of Transients</b>	1	<b>Original Points Count</b>	8124	<b>Frequency (MHz)</b>	300.13	
<b>Pulse Sequence</b>	zq	<b>Solvent</b>	CHLOROFORM-D		<b>Points Count</b>	8192	<b>Sweep Width (Hz)</b>	7500.00
<b>Temperature (degree C)</b>	22.500							



**5d**



No.	Annotation	(ppm)
1	Chloroform-d	7.25

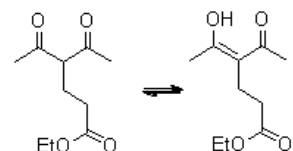
No.	(ppm)	Value
1	.03 .. 4.3	100.000
2	.58 .. 16.	0.604

<sup>13</sup>C NMR of ethyl 4-acetyl-5-oxohexanoate (**5d**)

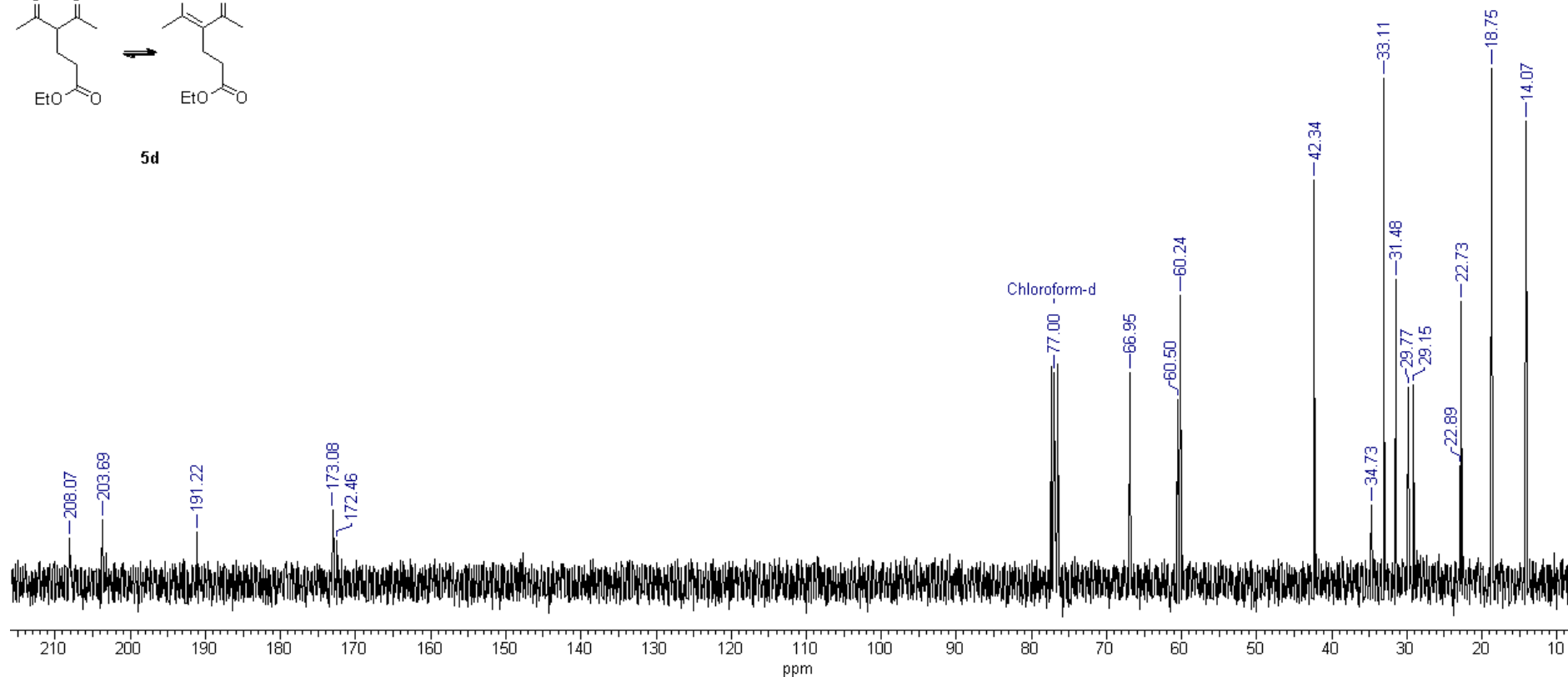
Acquisition Time (sec) 0.4501

Date 21 Sep 2013 08:36:16  
 Frequency (MHz) 75.48  
 Points Count 16384  
 Sweep Width (Hz) 18115.94

Nucleus 13C  
 Pulse Sequence zgpg baseopt  
 Temperature (degree C) 22.800  
 Number of Transients 122  
 Solvent CHLOROFORM-D  
 Original Points Count 16308



**5d**

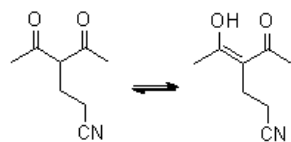


No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	14.07	1062.3	0.8975	8	33.11	2498.7	0.9795	15	172.46	13016.9	0.0812
2	18.75	1415.1	1.0000	9	34.73	2621.5	0.1495	16	173.08	13063.3	0.1399
3	22.73	1715.8	0.5460	10	42.34	3195.4	0.7825	17	191.22	14432.3	0.0968
4	22.89	1728.0	0.2275	11	60.24	4546.6	0.5586	18	203.69	15373.3	0.1230
5	29.15	2200.2	0.3838	12	60.50	4566.5	0.3559	19	208.07	15703.9	0.0853
6	29.77	2246.6	0.3791	13	66.95	5053.1	0.4085				
7	31.48	2376.0	0.5891	14	77.00	5811.6	0.4076				

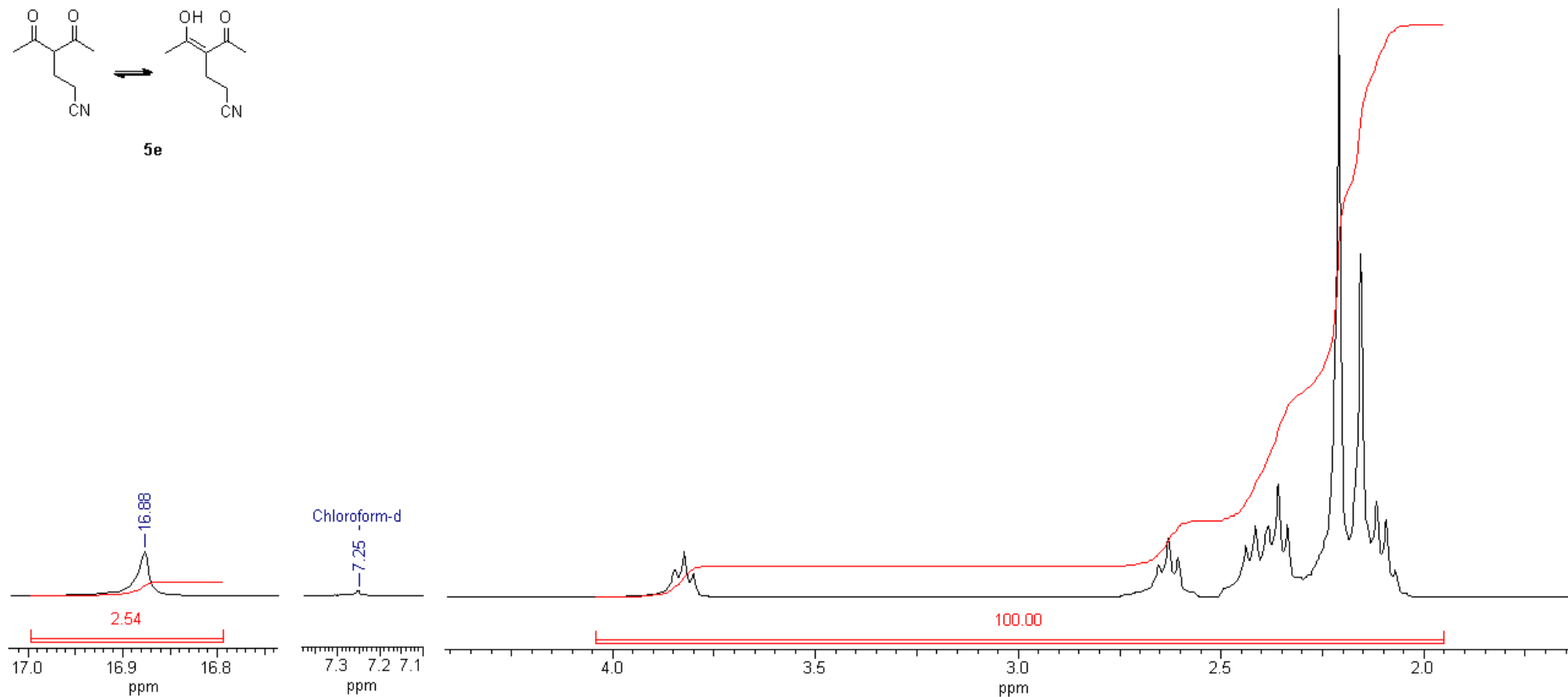
No.	Annotation	(ppm)
1	Chloroform-d	77.00

<sup>1</sup>H NMR of 4-acetyl-5-oxohexanenitrile (**5e**)

<b>Acquisition Time (sec)</b>	0.6759	<b>Comment</b>	NMR/50561344	<b>Date</b>	23 Sep 2013 11:41:52
<b>Nucleus</b>	1H	<b>Number of Transients</b>	1	<b>Original Points Count</b>	8124
<b>Pulse Sequence</b>	zg	<b>Solvent</b>	CHLOROFORM-D	<b>Points Count</b>	8192
<b>Temperature (degree C)</b>	23.700			<b>Sweep Width (Hz)</b>	6009.62



**5e**



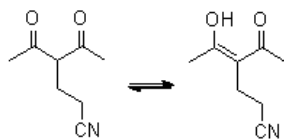
No.	(ppm)	(Hz)	Height
1	7.25	2176.0	0.0079
2	16.88	5065.2	0.0751

No.	Annotation	(ppm)
1	Chloroform-d	7.25

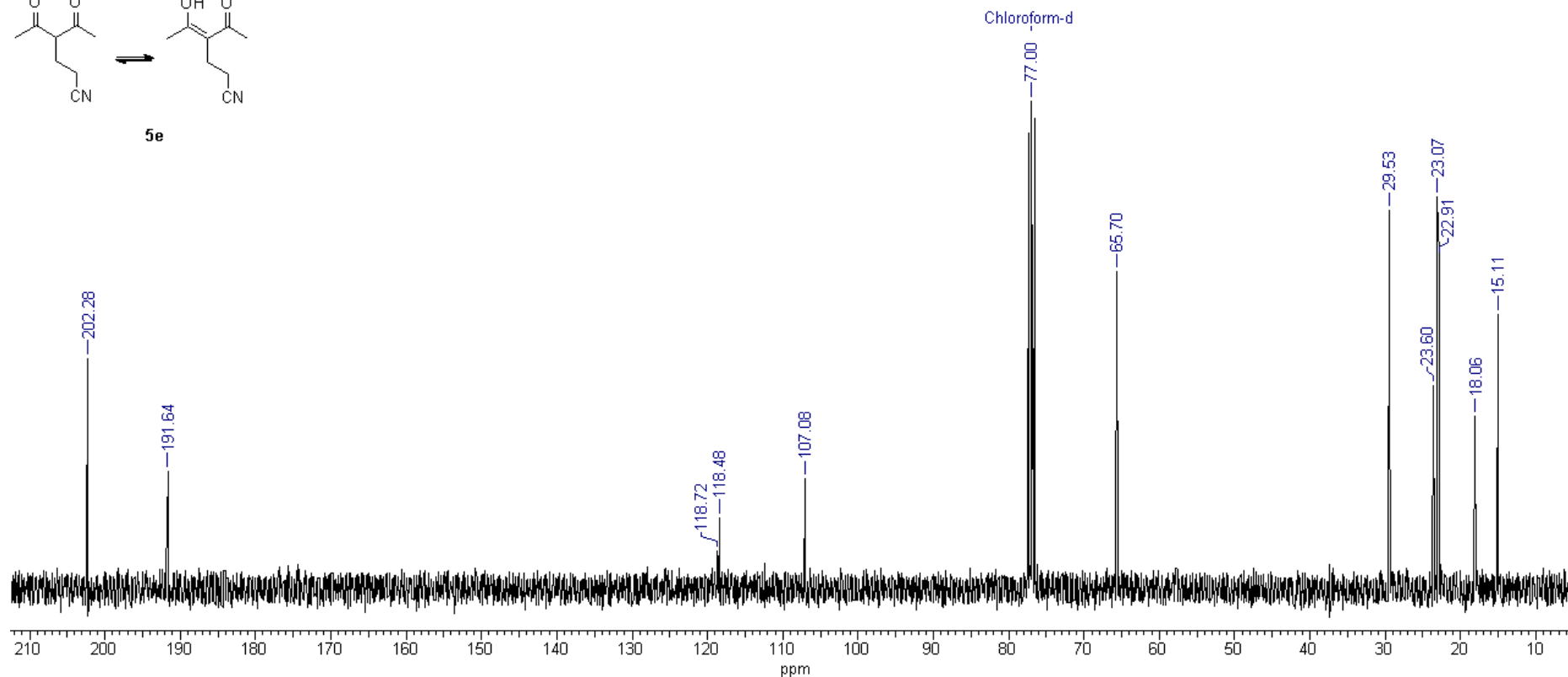
No.	(ppm)	Value
1	.95 .. 4.0	100.000
2	.79 .. 17.	2.541

<sup>13</sup>C NMR of 4-acetyl-5-oxohexanenitrile (**5e**)

<b>Acquisition Time (sec)</b> 0.4503		<b>Date</b> 23 Sep 2013 11:44:00	
<b>Nucleus</b> 13C	<b>Number of Transients</b> 274	<b>Original Points Count</b> 16316	<b>Frequency (MHz)</b> 75.48
<b>Pulse Sequence</b> zgpg30	<b>Solvent</b> CHLOROFORM-D	<b>Points Count</b> 16384	<b>Sweep Width (Hz)</b> 18115.94
<b>Temperature (degree C)</b> 23.700			



**5e**



No.	(ppm)	(Hz)	Height
1	15.11	1140.8	0.5630
2	18.06	1363.1	0.3546
3	22.91	1729.1	0.6817
4	23.07	1741.3	0.8040
5	23.60	1781.1	0.4178
6	29.53	2228.9	0.7756
7	65.70	4959.1	0.6501

No.	(ppm)	(Hz)	Height
8	77.00	5811.6	1.0000
9	107.08	8081.8	0.2254
10	118.48	8942.1	0.1463
11	118.72	8960.9	0.0795
12	191.64	14464.3	0.2430
13	202.28	15267.1	0.4730

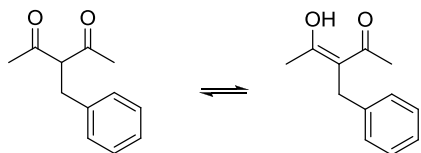
No.	Annotation	(ppm)
1	Chloroform-d	77.00

<sup>1</sup>H NMR of 3-benzylpentane-2,4-dione (**5f**)

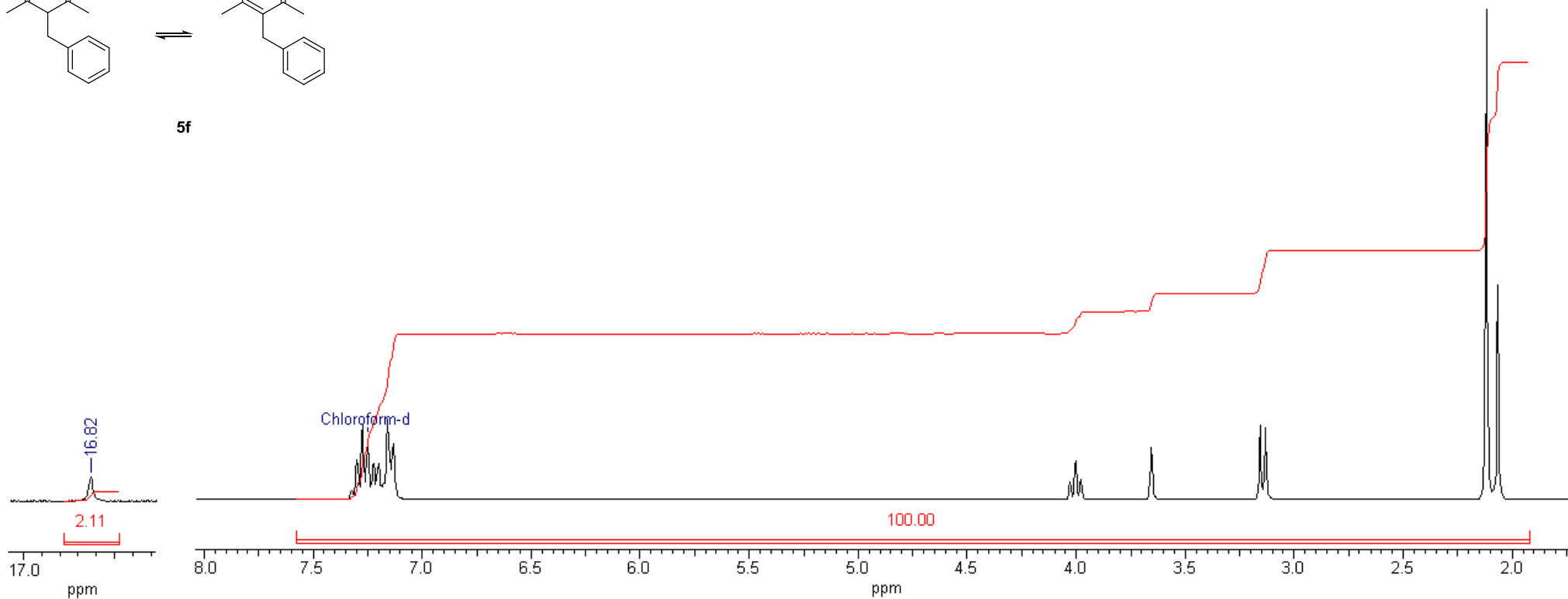
Acquisition Time (sec) 0.6759

Date 17 Sep 2013 14:00:32

Number of Transients	1	Original Points Count	8124	Points Count	8192	Frequency (MHz)	300.13	Nucleus	1H
Solvent	CHLOROFORM-D	Sweep Width (Hz)	6009.62	Pulse Sequence	zg	Temperature (degree C)	23.500		



**5f**



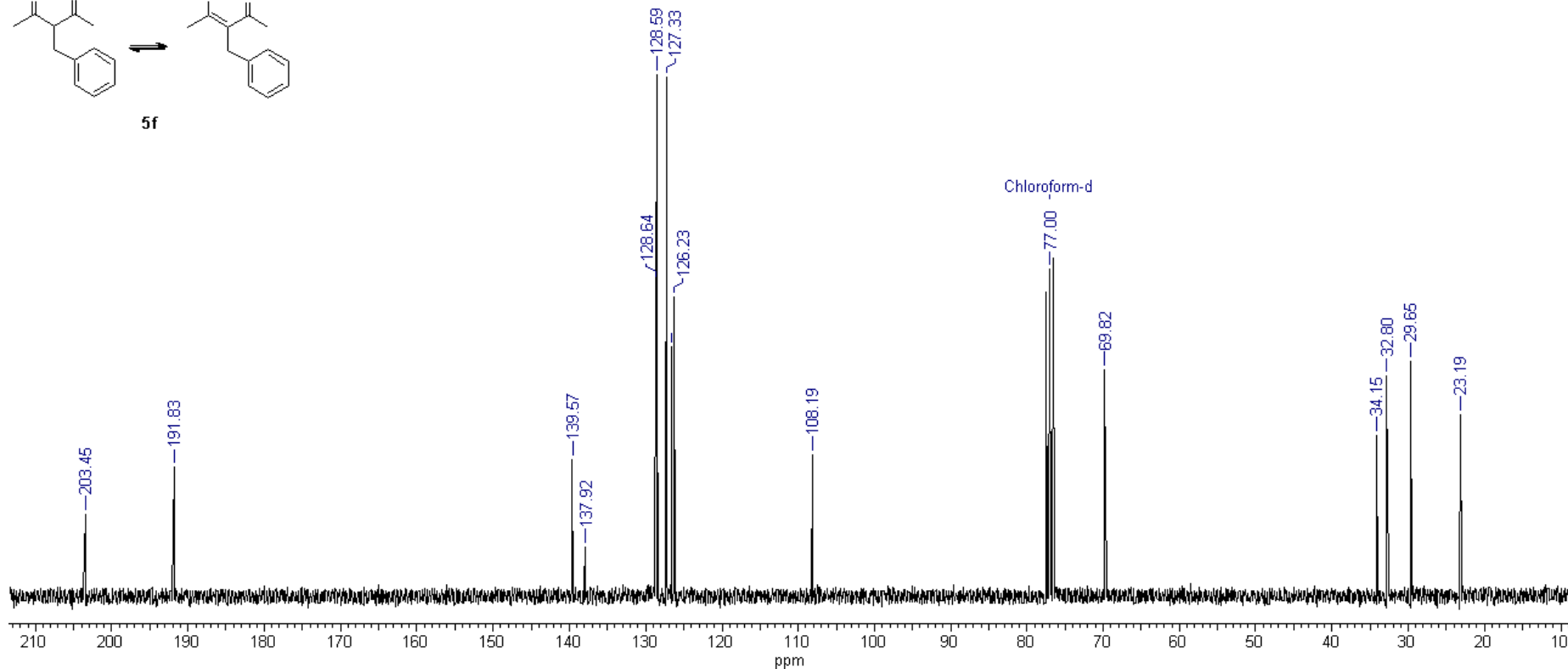
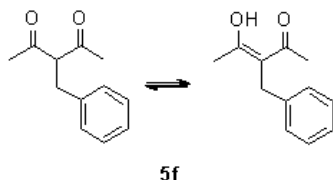
No.	(ppm)	(Hz)	Height
1	16.82	5046.8	0.0467

No.	Annotation	(ppm)
1	Chloroform-d	7.25

No.	(ppm)	Value
1	92 .. 7.5	100.000
2	74 .. 16.	2.110

<sup>13</sup>C NMR of 3-benzylpentane-2,4-dione (**5f**)

<b>Acquisition Time (sec)</b> 0.4503		<b>Date</b> 23 Sep 2013 14:09:04	
<b>File Name</b>		<b>Frequency (MHz)</b> 75.48	
<b>Nucleus</b> 13C	<b>Number of Transients</b> 298	<b>Original Points Count</b> 16316	<b>Points Count</b> 16384
<b>Pulse Sequence</b> zgpg30	<b>Solvent</b> CHLOROFORM-D	<b>Sweep Width (Hz)</b> 18115.94	
<b>Temperature (degree C)</b> 23.400			

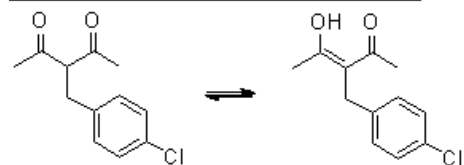


No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	23.19	1750.2	0.3482	10	127.33	9610.0	0.9943
2	29.65	2237.8	0.4507	11	128.51	9699.6	0.4819
3	32.80	2475.6	0.4213	12	128.59	9705.1	1.0000
4	34.15	2577.3	0.3083	13	128.64	9709.6	0.6033
5	69.82	5269.9	0.4339	14	137.92	10409.5	0.0943
6	77.00	5811.7	0.6263	15	139.57	10534.5	0.2618
7	108.19	8165.9	0.2701	16	191.83	14478.8	0.2467
8	126.23	9527.1	0.5736	17	203.45	15355.7	0.1568
9	126.67	9560.3	0.4780				

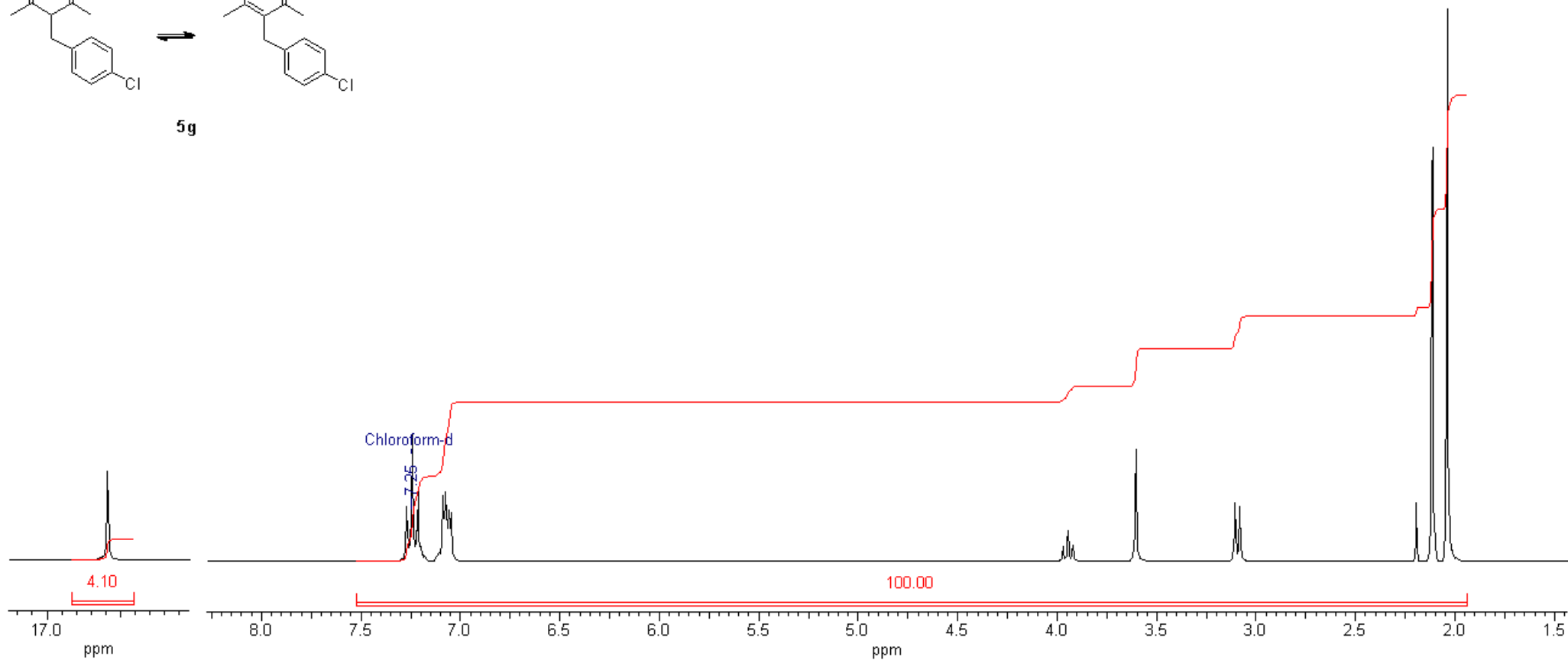
No.	Annotation	(ppm)
1	Chloroform-d	77.00

### <sup>1</sup>H NMR of 3-(4-chlorobenzyl)pentane-2,4-dione (**5g**)

<b>Acquisition Time (sec)</b> 0.6759			<b>Date</b> 23 Sep 2013 11:18:24	
<b>Nucleus</b> 1H	<b>Number of Transients</b> 1	<b>Original Points Count</b> 8124	<b>Frequency (MHz)</b> 300.13	
<b>Pulse Sequence</b> zg	<b>Solvent</b> CHLOROFORM-D		<b>Points Count</b> 8192	
<b>Temperature (degree C)</b> 23.500			<b>Sweep Width (Hz)</b> 6009.62	



**5g**



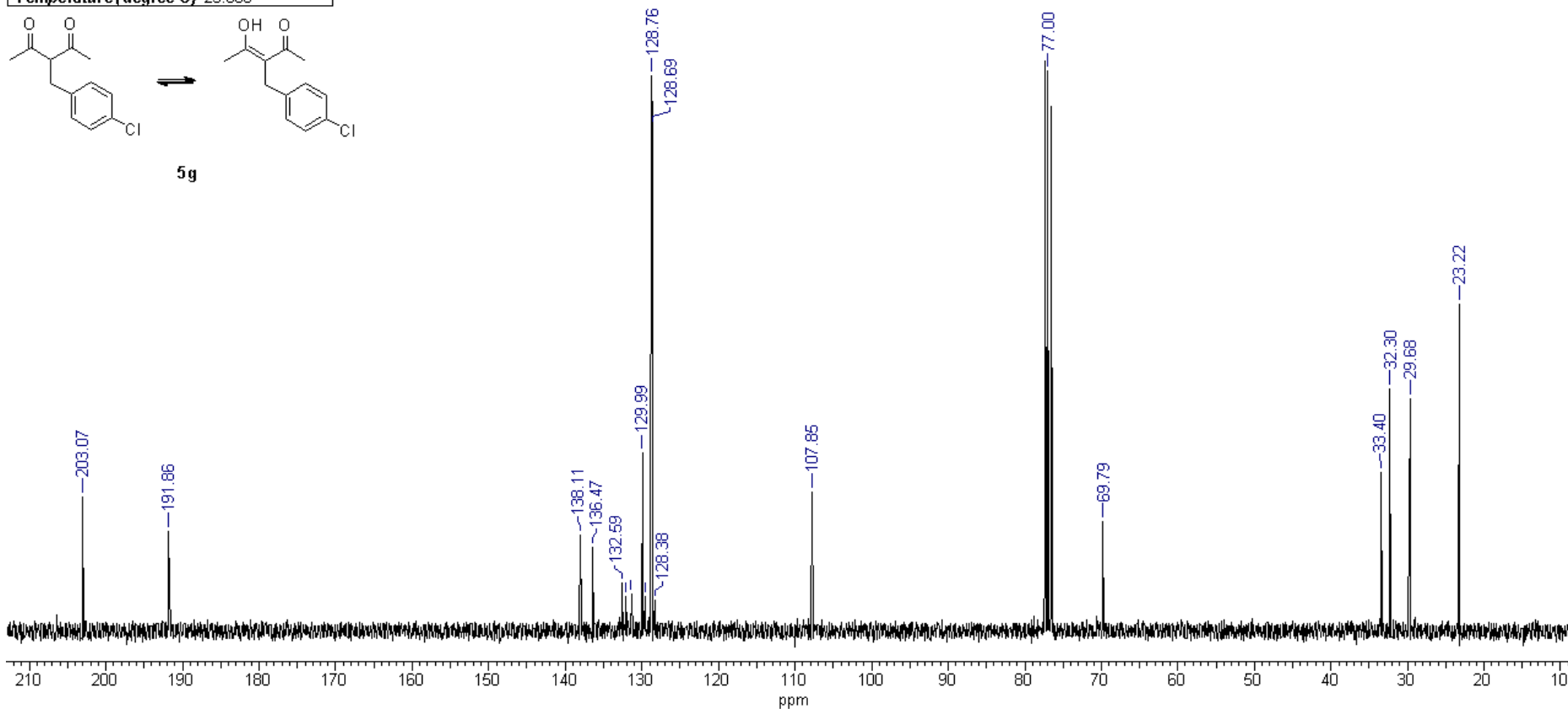
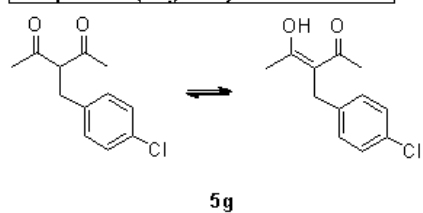
No.	(ppm)	(Hz)	Height
1	7.25	2176.0	0.0847

No.	Annotation	(ppm)
1	Chloroform-d	7.25

No.	(ppm)	Value
1	94 .. 7.5	100.000
2	71 .. 16	4.099

<sup>13</sup>C NMR of 3-(4-chlorobenzyl)pentane-2,4-dione (**5g**)

<b>Acquisition Time (sec)</b> 0.4503		<b>Date</b> 23 Sep 2013 11:18:24	
<b>Nucleus</b> 13C	<b>Number of Transients</b> 608	<b>Original Points Count</b> 16316	<b>Frequency (MHz)</b> 75.48
<b>Pulse Sequence</b> zgpg30	<b>Solvent</b> CHLOROFORM-D	<b>Points Count</b> 16384	<b>Sweep Width (Hz)</b> 18115.94
<b>Temperature (degree C)</b> 23.600			

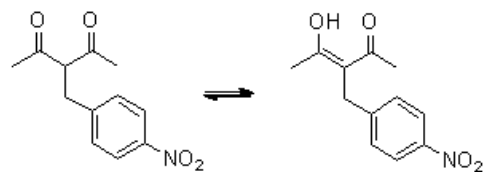


No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	23.22	1752.4	0.5732	8	128.38	9689.6	0.0552	15	131.40	9917.4	0.0656
2	29.68	2240.0	0.4075	9	128.51	9699.6	0.0510	16	132.06	9967.2	0.0622
3	32.30	2438.0	0.4257	10	128.69	9712.9	0.8850	17	132.59	10007.0	0.0840
4	33.40	2520.9	0.2792	11	128.76	9718.4	0.9728	18	136.47	10300.0	0.1476
5	69.79	5267.6	0.1922	12	128.81	9721.7	0.1979	19	138.11	10423.9	0.1690
6	77.00	5811.7	0.9605	13	129.65	9785.8	0.0606	20	191.86	14481.0	0.1756
7	107.85	8140.4	0.2438	14	129.99	9811.3	0.3117	21	203.07	15326.9	0.2364

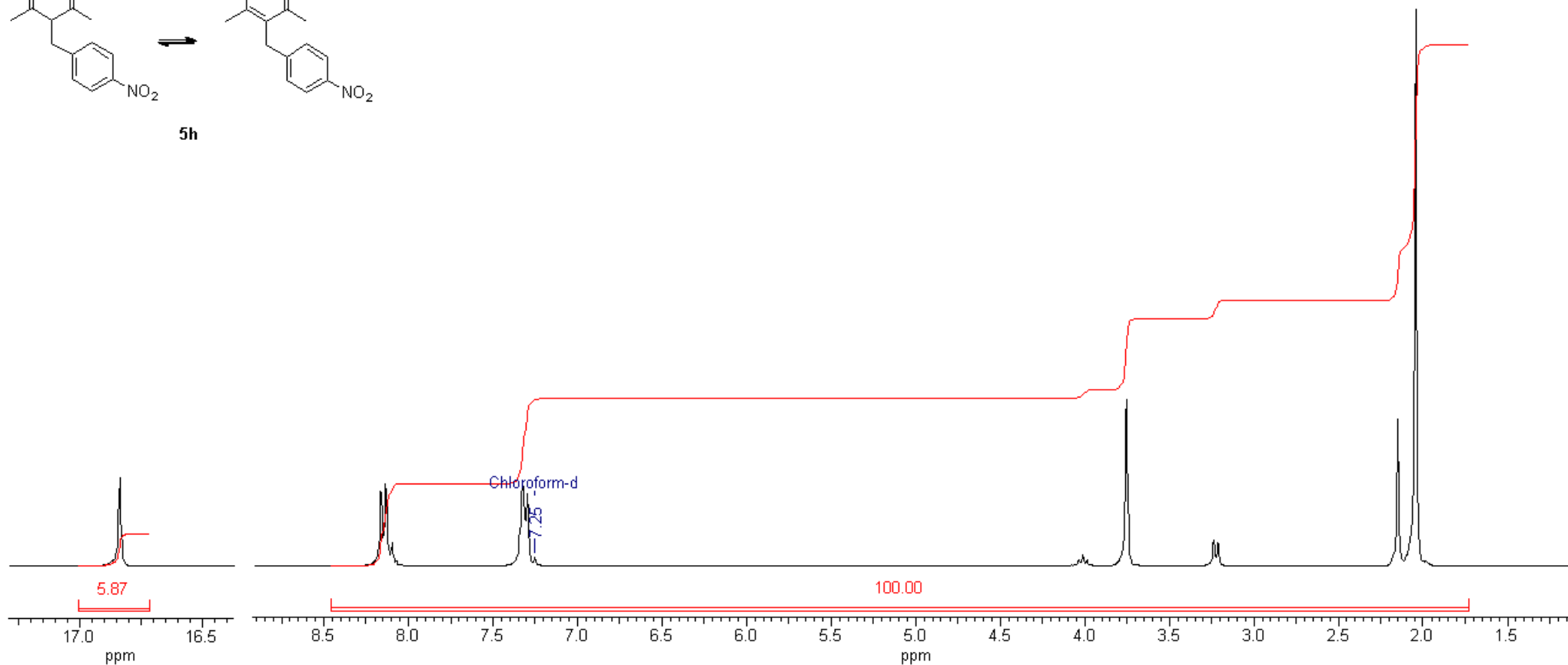


### <sup>1</sup>H NMR of 3-(4-nitrobenzyl)pentane-2,4-dione (**5h**)

<b>Acquisition Time (sec)</b> 0.6759	<b>Date</b> 23 Sep 2013 14:21:52			<b>Frequency (MHz)</b> 300.13
<b>Nucleus</b> 1H	<b>Number of Transients</b> 1	<b>Original Points Count</b> 8124	<b>Points Count</b> 8192	
<b>Pulse Sequence</b> zg	<b>Solvent</b> CHLOROFORM-D		<b>Sweep Width (Hz)</b> 6009.62	
<b>Temperature (degree C)</b> 23.800				



**5h**



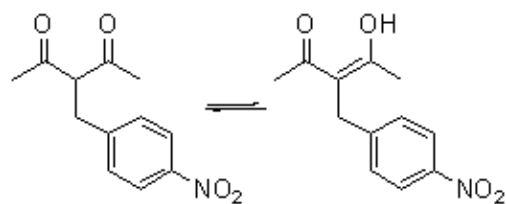
No.	(ppm)	(Hz)	Height
1	7.25	2176.0	0.0151

No.	Annotation	(ppm)
1	Chloroform-d	7.25

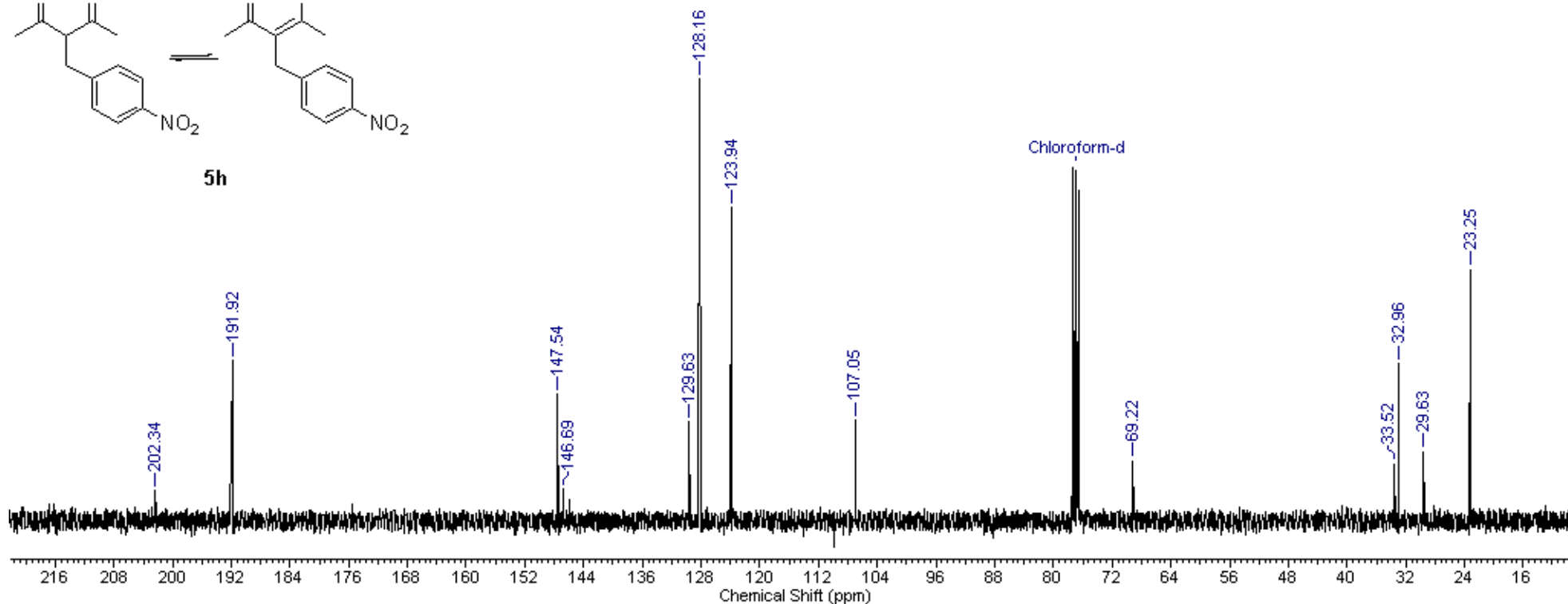
No.	(ppm)	Value
1	7.3 .. 8.4	100.000
2	7.1 .. 17.1	5.869

<sup>13</sup>C NMR of 3-(4-nitrobenzyl)pentane-2,4-dione (**5h**)

<b>Acquisition Time (sec)</b>	0.9006	<b>Date</b>	23 Sep 2013 14:21:52		
<b>Nucleus</b>	13C	<b>Number of Transients</b>	211	<b>Original Points Count</b>	16316
<b>Pulse Sequence</b>	zgpg30	<b>Solvent</b>	CHLOROFORM-D	<b>Sweep Width (Hz)</b>	18115.94
				<b>Frequency (MHz)</b>	75.48
				<b>Points Count</b>	16384
				<b>Temperature (degree C)</b>	23.600



**5h**

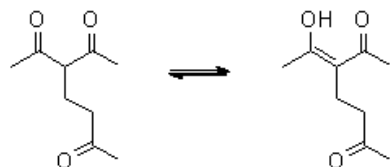


No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	23.25	1754.6	0.5657	8	123.94	9354.6	0.7055
2	29.63	2236.7	0.1509	9	128.16	9673.0	1.0000
3	32.96	2487.7	0.3503	10	129.63	9783.6	0.2177
4	33.52	2529.7	0.1232	11	146.69	11071.8	0.0631
5	69.22	5224.5	0.1295	12	147.54	11136.0	0.2797
6	107.05	8079.6	0.2220	13	191.92	14485.4	0.3576
7	123.84	9346.8	0.2620	14	202.34	15271.6	0.0605

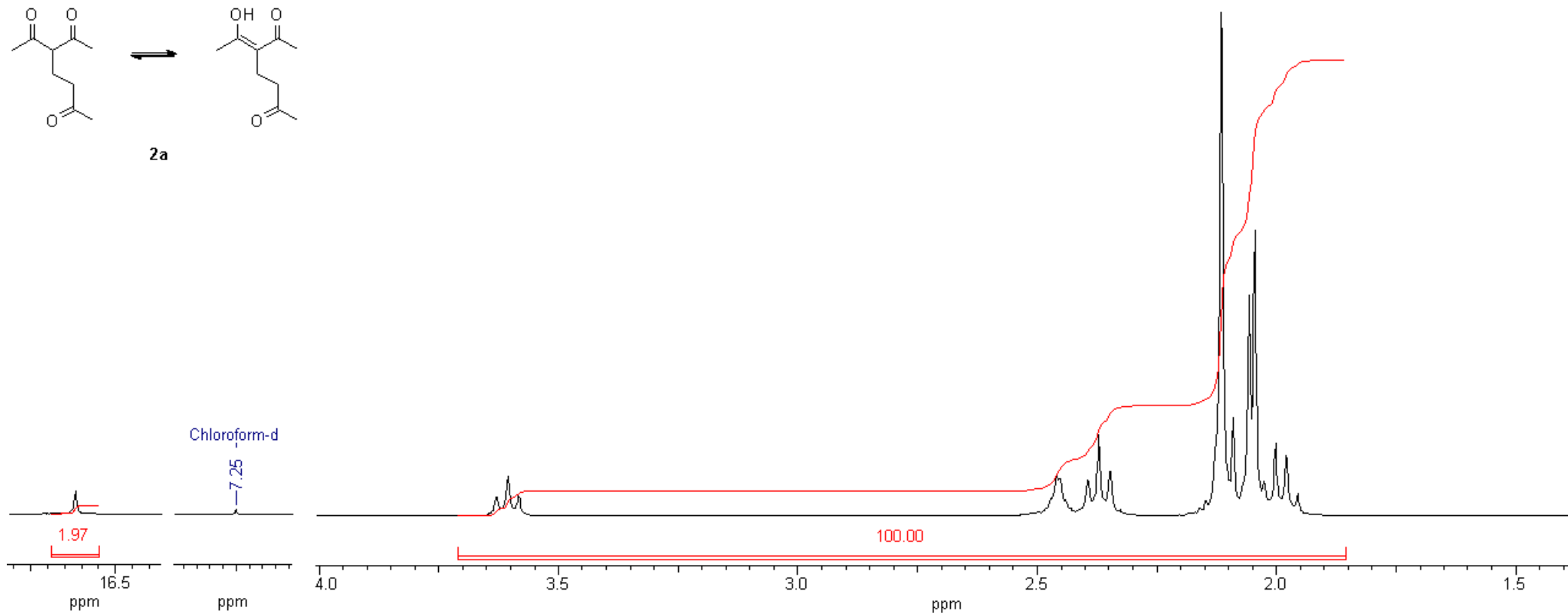
No.	Annotation	(ppm)
1	Chloroform-d	77.00

### <sup>1</sup>H NMR of 3-acetylheptane-2,6-dione (2a)

<b>Acquisition Time (sec)</b> 0.6759			<b>Date</b> 17 Jun 2013 15:25:52	
<b>Nucleus</b> 1H	<b>Number of Transients</b> 1	<b>Original Points Count</b> 8124	<b>Frequency (MHz)</b> 300.13	<b>Points Count</b> 8192
<b>Pulse Sequence</b> zg	<b>Solvent</b> CHLOROFORM-D		<b>Sweep Width (Hz)</b> 6009.62	
<b>Temperature (degree C)</b> 26.900				



2a



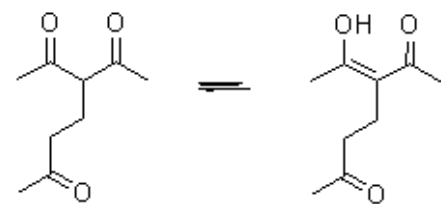
No.	(ppm)	(Hz)	Height
1	7.25	2176.0	0.0107

No.	Annotation	(ppm)
1	Chloroform-d	7.25

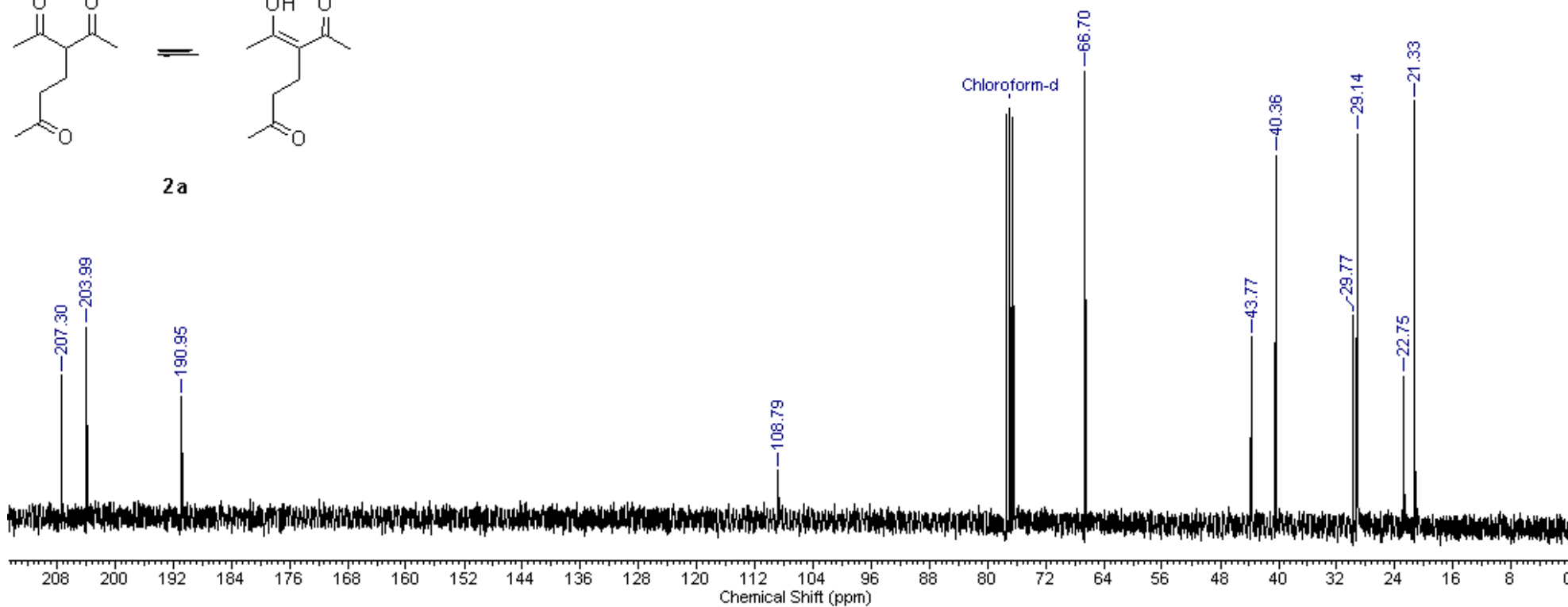
No.	(ppm)	Value
1	86 .. 3.7	100.000
2	55 .. 16.	1.969

<sup>13</sup>C NMR of 3-acetylheptane-2,6-dione (2a)

<b>Acquisition Time (sec)</b>	0.9006	<b>Date</b>	17 Jun 2013 15:28:00			
<b>Nucleus</b>	13C	<b>Number of Transients</b>	181	<b>Original Points Count</b>	16316	
<b>Pulse Sequence</b>	zgpg30	<b>Solvent</b>	CHLOROFORM-D	<b>Sweep Width (Hz)</b>	18115.94	
					<b>Frequency (MHz)</b>	75.48
					<b>Points Count</b>	16384
					<b>Temperature (degree C)</b>	26.900



2a

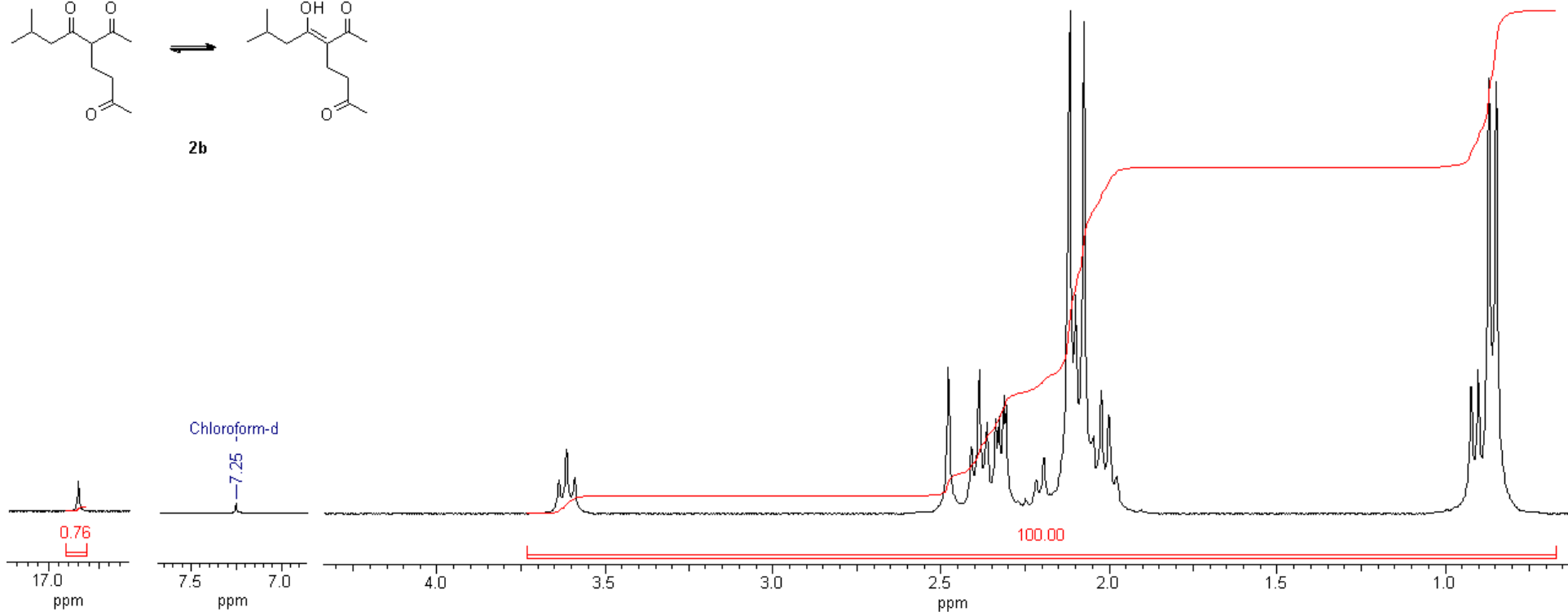
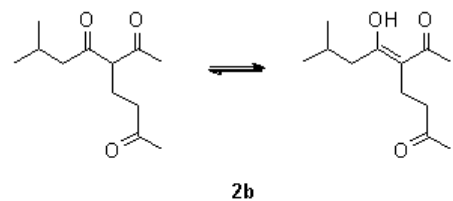


No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	21.25	1604.2	0.2815	8	43.77	3303.8	0.4426
2	21.33	1609.7	0.9371	9	66.70	5034.3	1.0000
3	22.75	1717.0	0.3619	10	108.79	8211.2	0.1643
4	29.14	2199.1	0.8693	11	190.95	14412.4	0.3187
5	29.77	2246.6	0.4886	12	203.99	15396.5	0.4639
6	29.90	2256.6	0.1926	13	207.30	15646.4	0.3639
7	40.36	3046.1	0.8239				

No.	Annotation	(ppm)
1	Chloroform-d	77.00

### <sup>1</sup>H NMR of 5-acetyl-8-methylnonane-2,6-dione (2b)

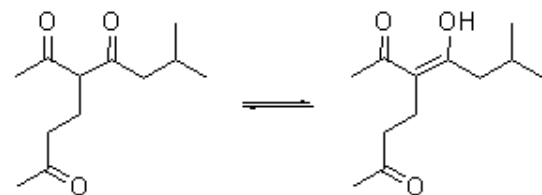
<b>Acquisition Time (sec)</b> 0.6759			<b>Date</b> 27 Feb 2013 15:02:24	
<b>Nucleus</b> 1H	<b>Number of Transients</b> 1	<b>Original Points Count</b> 8124	<b>Frequency (MHz)</b> 300.13	
<b>Pulse Sequence</b> zg	<b>Solvent</b> CHLOROFORM-D		<b>Points Count</b> 8192	
<b>Temperature (degree C)</b> 26.700			<b>Sweep Width (Hz)</b> 6009.62	



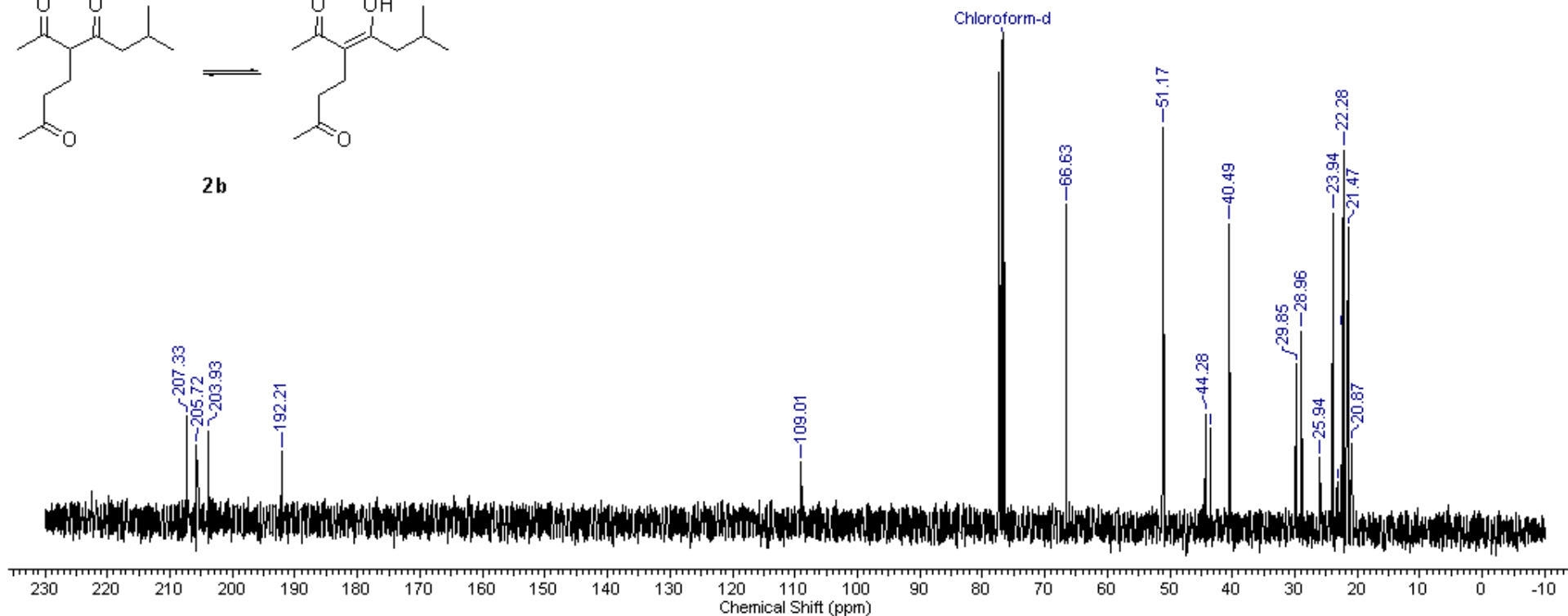
No.	(ppm)	(Hz)	Height	No.	Annotation	(ppm)	No.	(ppm)	Value
1	7.25	2176.0	0.0198	1	Chloroform-d	7.25	1	67 ... 3.7	100.000
							2	81 ... 16	0.759

<sup>13</sup>C NMR of 5-acetyl-8-methylnonane-2,6-dione (**2b**)

<b>Acquisition Time (sec)</b>	0.9006	<b>Comment</b>	Avance-300, C-13, CDCl3		<b>Date</b>	27 Feb 2013 15:04:32	
<b>Nucleus</b>	13C	<b>Number of Transients</b>	195	<b>Original Points Count</b>	16316	<b>Frequency (MHz)</b>	75.48
<b>Pulse Sequence</b>	zgpg30	<b>Solvent</b>	CHLOROFORM-D	<b>Sweep Width (Hz)</b>	18115.94	<b>Points Count</b>	16384
						<b>Temperature (degree C)</b>	26.700



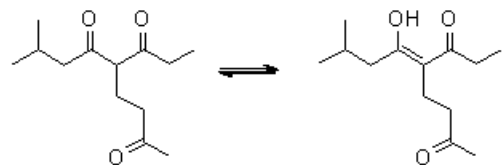
**2b**



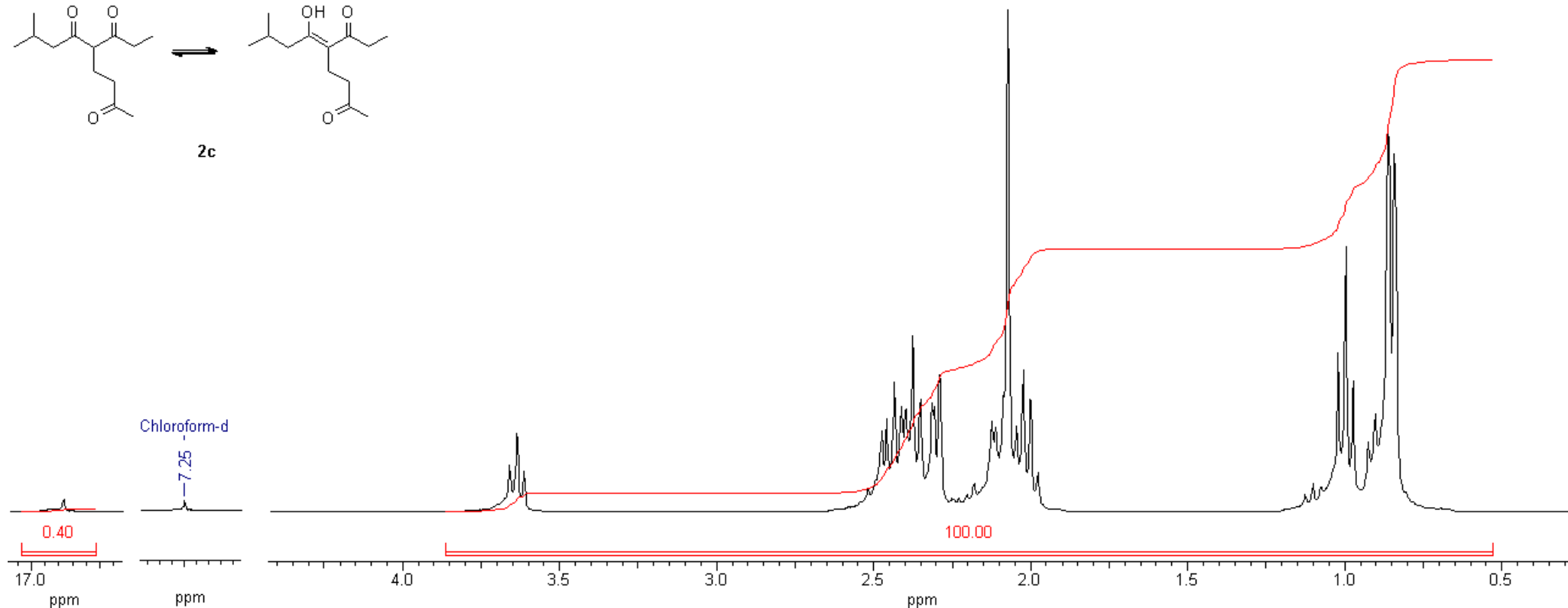
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	Annotation	(ppm)
1	20.87	1575.4	0.1683	12	40.49	3056.1	0.6130	1	Chloroform-d	77.00
2	21.47	1620.8	0.6042	13	43.57	3288.3	0.1985			
3	22.28	1681.6	0.7624	14	44.28	3342.5	0.2277			
4	22.34	1686.0	0.4865	15	51.17	3862.2	0.8090			
5	22.56	1702.6	0.3998	16	66.63	5028.8	0.6510			
6	23.26	1755.7	0.0880	17	109.01	8227.8	0.1286			
7	23.94	1806.5	0.6353	18	192.21	14507.5	0.1519			
8	25.94	1958.0	0.1376	19	203.93	15392.1	0.1936			
9	28.96	2185.8	0.3951	20	205.72	15527.0	0.1627			
10	29.85	2253.3	0.3274	21	207.33	15648.6	0.2228			
11	29.96	2261.0	0.1158							

<sup>1</sup>H NMR of 8-methyl-5-propionylnonane-2,6-dione (**2c**)

<b>Acquisition Time (sec)</b>	0.6759	<b>Comment</b>	Avance-300, 1H CDCl3	<b>Date</b>	08 Dec 2012 11:58:56
<b>Nucleus</b>	1H	<b>Number of Transients</b>	1	<b>Original Points Count</b>	8124
<b>Pulse Sequence</b>	zg	<b>Solvent</b>	CHLOROFORM-D	<b>Frequency (MHz)</b>	300.13
<b>Temperature (degree C)</b>	27.900			<b>Points Count</b>	8192
				<b>Sweep Width (Hz)</b>	6009.62



**2c**



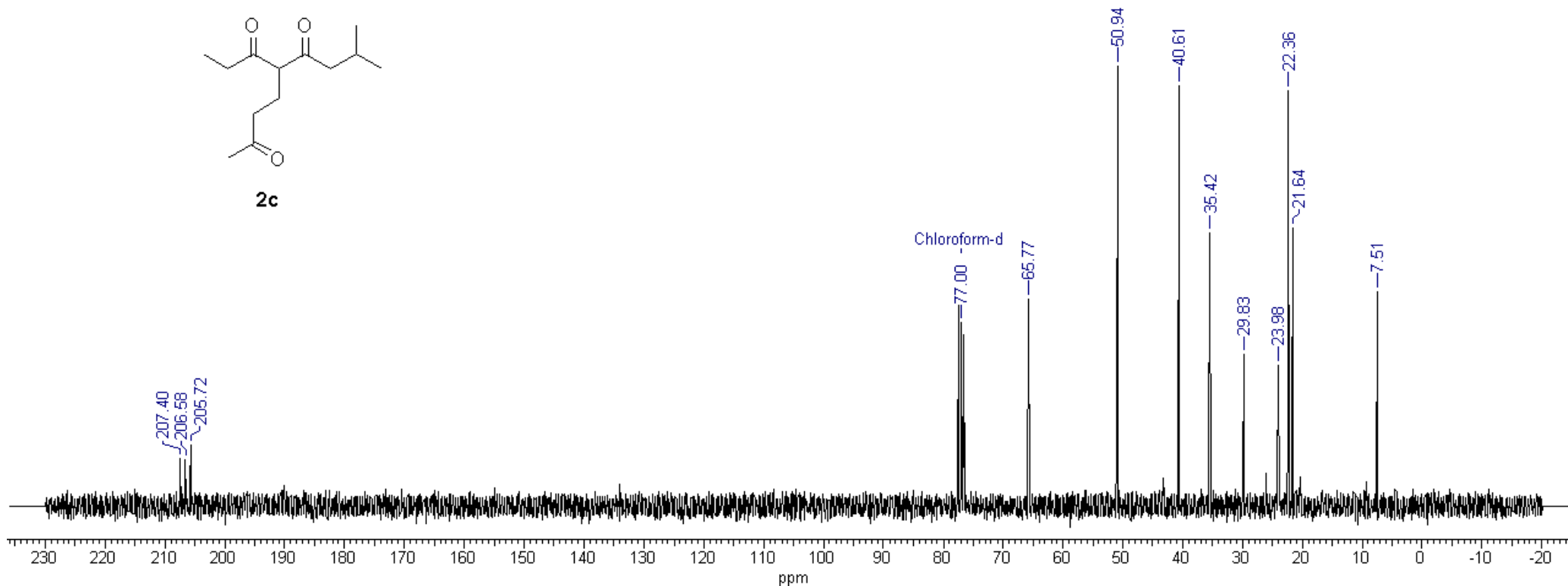
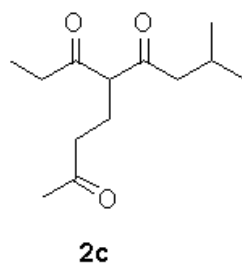
No.	(ppm)	(Hz)	Height
1	7.25	2175.9	0.0207

No.	Annotation	(ppm)
1	Chloroform-d	7.25

No.	(ppm)	Value
1	53 .. 3.8	100.000
2	7.6 .. 17.	0.401

<sup>13</sup>C NMR of 8-methyl-5-propionylnonane-2,6-dione (**2c**)

<b>Acquisition Time (sec)</b> 0.4322		<b>Date</b> 08 Dec 2012 12:03:12		<b>Frequency (MHz)</b> 75.48
<b>Nucleus</b> 13C	<b>Number of Transients</b> 193	<b>Original Points Count</b> 16308	<b>Points Count</b> 16384	
<b>Pulse Sequence</b> zgpg60base	<b>Solvent</b> CHLOROFORM-D	<b>Sweep Width (Hz)</b> 18867.92		
<b>Temperature (degree C)</b> 28.200				

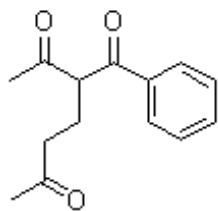


No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	Annotation	(ppm)
1	7.51	566.9	0.4857	8	50.94	3844.6	1.0000	1	Chloroform-d	77.00
2	21.64	1633.3	0.6324	9	65.77	4964.0	0.4701			
3	22.36	1687.5	0.9433	10	77.00	5811.6	0.4146			
4	23.98	1809.5	0.3192	11	205.72	15527.2	0.1386			
5	29.83	2251.8	0.3423	12	206.58	15591.7	0.1053			
6	35.42	2673.3	0.6191	13	207.40	15653.9	0.1066			
7	40.61	3064.9	0.9548							

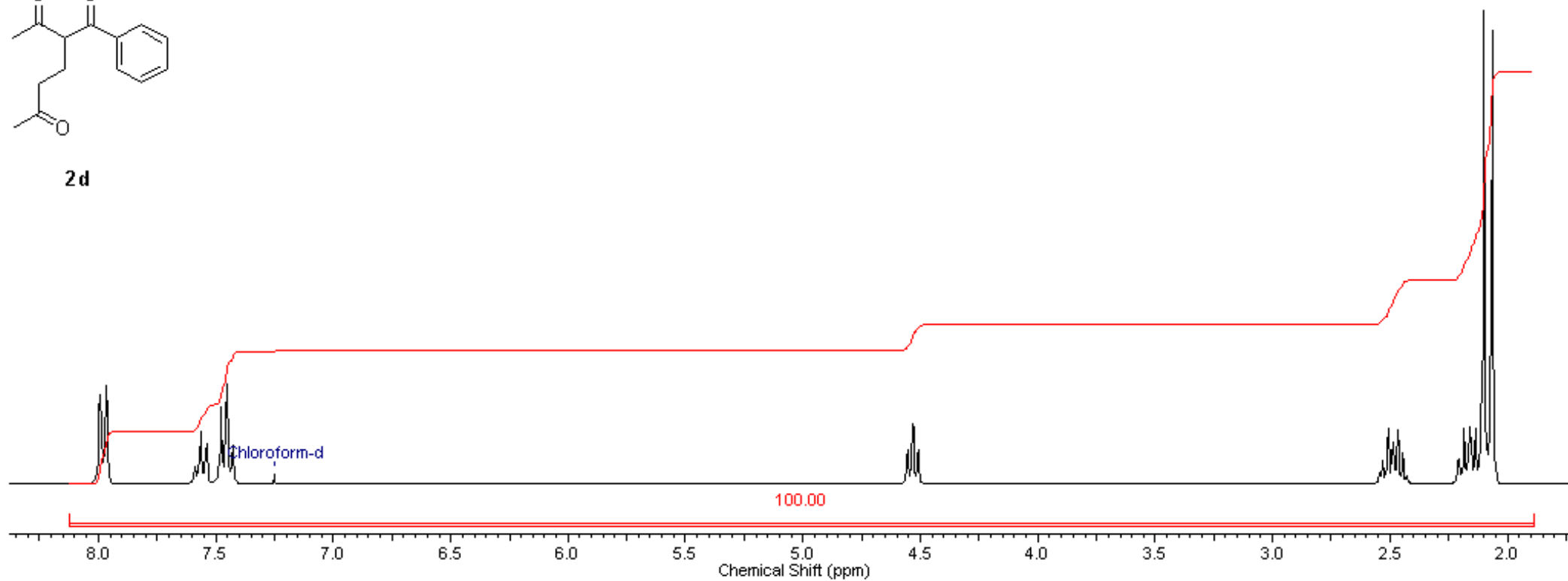


<sup>1</sup>H NMR of 3-benzoylheptane-2,6-dione (**2d**)

<b>Acquisition Time (sec)</b>	1.3518	<b>Date</b>	04 Oct 2012 15:47:12	<b>Frequency (MHz)</b>	300.13		
<b>Nucleus</b>	1H	<b>Number of Transients</b>	1	<b>Original Points Count</b>	8124	<b>Points Count</b>	8192
<b>Pulse Sequence</b>	zg31	<b>Solvent</b>	CHLOROFORM-D	<b>Sweep Width (Hz)</b>	6009.62		
<b>Temperature (degree C)</b>	27.000						



**2d**



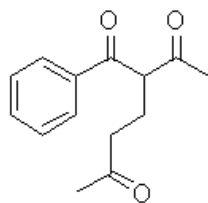
No.	Annotation	(ppm)	No.	(ppm)	Value	Absolute Value
1	Chloroform-d	7.25	1	[1.89 .. 8.13]	100.000	1.64613e+9

<sup>13</sup>C NMR of 3-benzoylheptane-2,6-dione (**2d**)

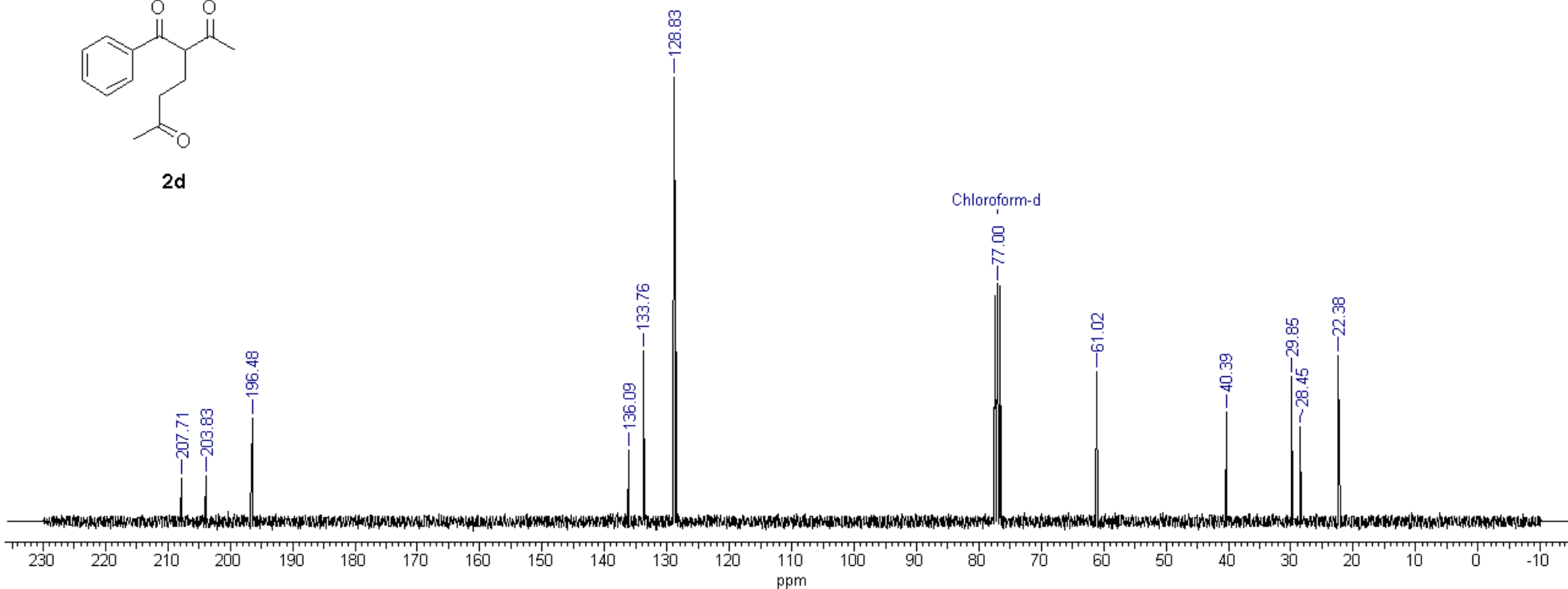
Acquisition Time (sec) 0.4501

Date 04 Oct 2012 15:49:20

Nucleus	13C	Number of Transients	139	Original Points Count	16308	Frequency (MHz)	75.48
Pulse Sequence	zgpg30base	Solvent	CHLOROFORM-D	Points Count	16384	Sweep Width (Hz)	18115.94
Temperature (degree C)	27.100						



**2d**



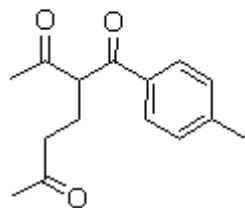
No.	(ppm)	(Hz)	Height
1	22.38	1689.3	0.3734
2	28.45	2147.1	0.2119
3	29.85	2253.3	0.3260
4	40.39	3048.3	0.2457
5	61.02	4605.3	0.3378
6	77.00	5811.7	0.5360
7	128.64	9709.5	0.7669

No.	(ppm)	(Hz)	Height
8	128.83	9723.9	1.0000
9	133.76	10095.4	0.3829
10	136.09	10271.3	0.1593
11	196.48	14829.3	0.2330
12	203.83	15384.4	0.1031
13	207.71	15677.4	0.0971

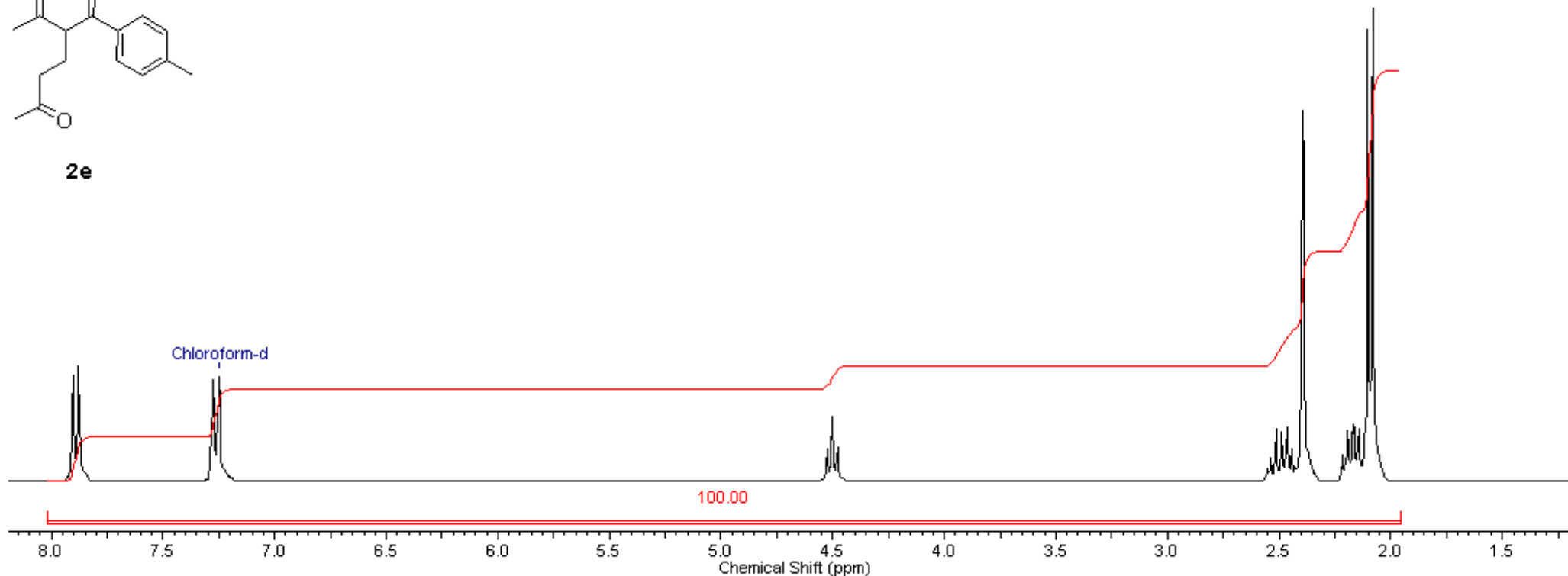
No.	Annotation	(ppm)
1	Chloroform-d	77.00

<sup>1</sup>H NMR of 3-(4-methylbenzoyl)heptane-2,6-dione (**2e**)

<b>Acquisition Time (sec)</b>	1.3518	<b>Date</b>	08 Oct 2012 12:18:08	<b>Frequency (MHz)</b>	300.13		
<b>Nucleus</b>	1H	<b>Number of Transients</b>	1	<b>Original Points Count</b>	8124	<b>Points Count</b>	8192
<b>Pulse Sequence</b>	zg	<b>Solvent</b>	CHLOROFORM-D	<b>Sweep Width (Hz)</b>	6009.62		
<b>Temperature (degree C)</b>	26.400						



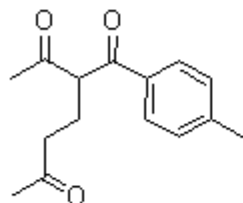
**2e**



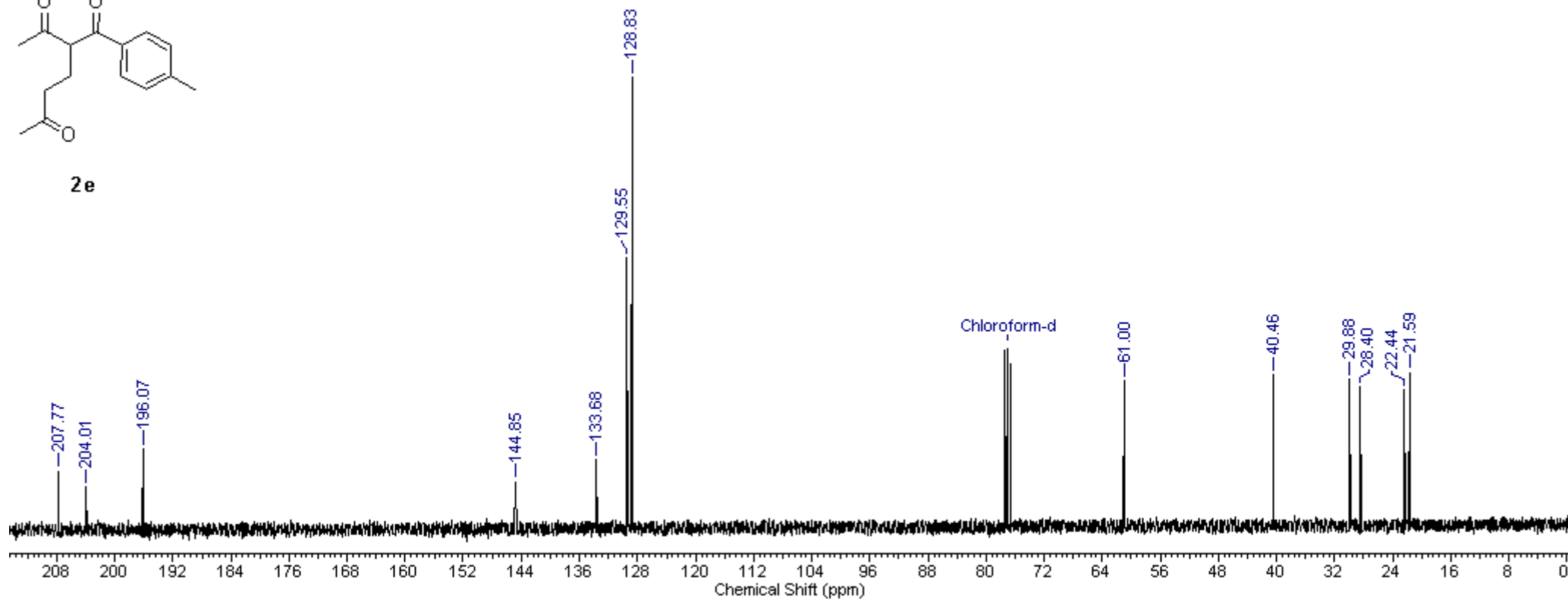
No.	Annotation	(ppm)	No.	(ppm)	Value	Absolute Value
1	Chloroform-d	7.25	1	[1.96 .. 8.02]	100.000	1.31456e+9

<sup>13</sup>C NMR of 3-(4-methylbenzoyl)heptane-2,6-dione (**2e**)

<b>Acquisition Time (sec)</b>	0.9006	<b>Date</b>	22 Jul 2013 11:16:16			
<b>Nucleus</b>	<sup>13</sup> C	<b>Number of Transients</b>	166	<b>Original Points Count</b>	16316	
<b>Pulse Sequence</b>	zgpg30	<b>Solvent</b>	CHLOROFORM-D	<b>Sweep Width (Hz)</b>	18115.94	
					<b>Frequency (MHz)</b>	75.48
					<b>Points Count</b>	16384
					<b>Temperature (degree C)</b>	27.300



**2e**



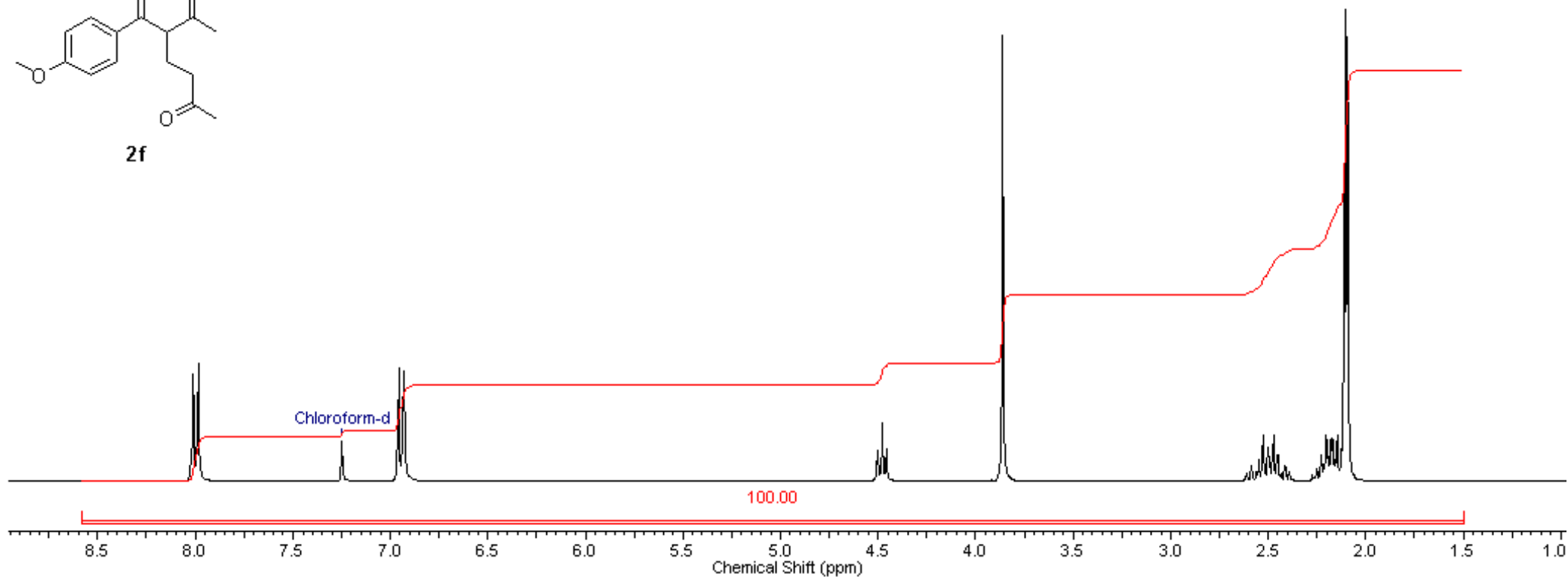
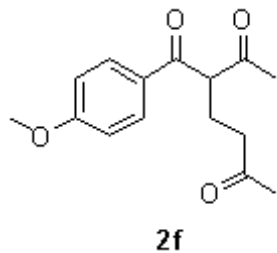
No.	(ppm)	(Hz)	Height
1	21.59	1629.6	0.3298
2	22.44	1693.7	0.2925
3	28.40	2143.8	0.2966
4	29.88	2255.5	0.3153
5	40.46	3053.8	0.3253
6	61.00	4604.1	0.3109
7	128.83	9723.9	1.0000

No.	(ppm)	(Hz)	Height
8	129.55	9778.1	0.5910
9	133.68	10089.9	0.1313
10	144.85	10932.5	0.0829
11	196.07	14798.3	0.1575
12	204.01	15397.6	0.0692
13	207.77	15681.8	0.1072

No.	Annotation	(ppm)
1	Chloroform-d	77.00

<sup>1</sup>H NMR of 3-(4-methoxybenzoyl)heptane-2,6-dione (**2f**)

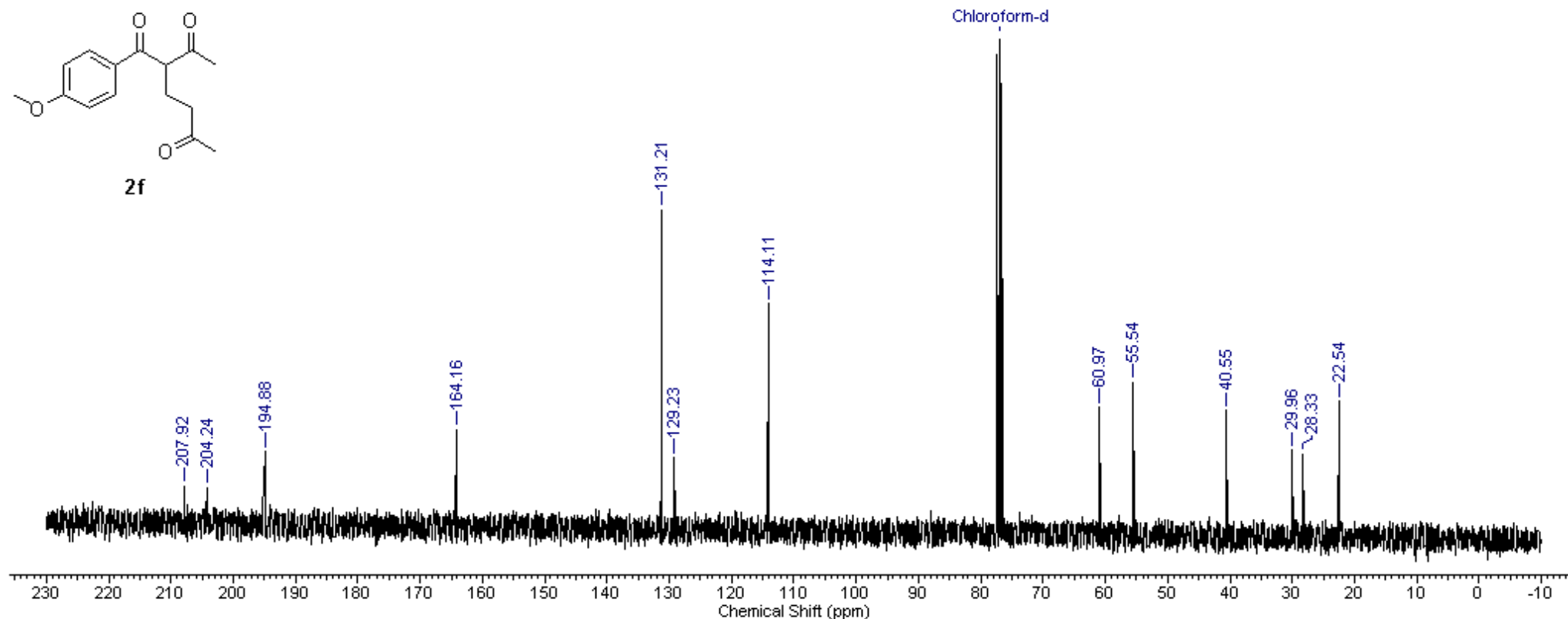
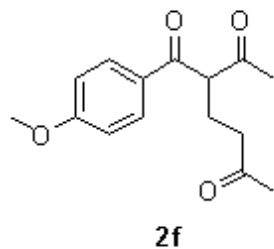
<b>Acquisition Time (sec)</b>	1.3518	<b>Date</b>	17 Jun 2013 11:14:08	<b>Frequency (MHz)</b>	300.13		
<b>Nucleus</b>	1H	<b>Number of Transients</b>	1	<b>Original Points Count</b>	8124	<b>Points Count</b>	8192
<b>Pulse Sequence</b>	zg31	<b>Solvent</b>	CHLOROFORM-D	<b>Sweep Width (Hz)</b>	6009.62		
<b>Temperature (degree C)</b>	26.900						



No.	Annotation	(ppm)	No.	(ppm)	Value	Absolute Value
1	Chloroform-d	7.25	1	[1.50 .. 8.58]	100.000	1.58319e+9

<sup>13</sup>C NMR of 3-(4-methoxybenzoyl)heptane-2,6-dione (**2f**)

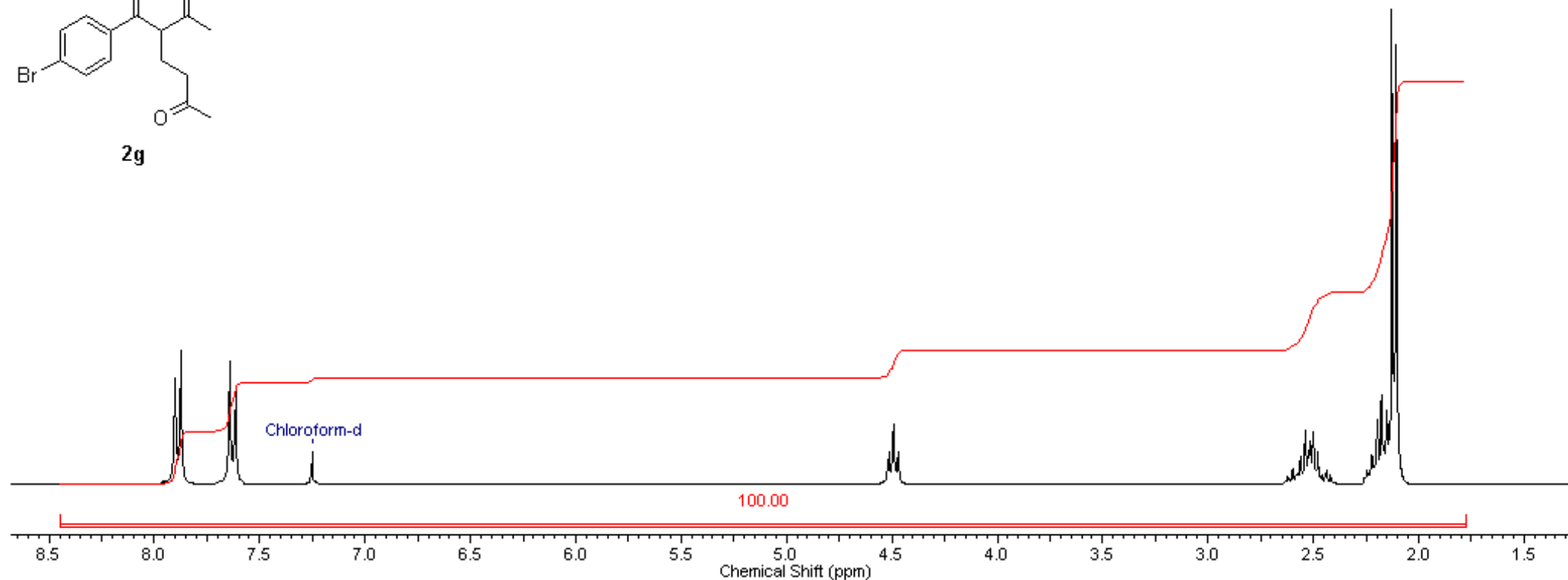
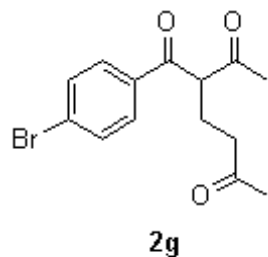
<b>Acquisition Time (sec)</b>	0.9006	<b>Date</b>	22 Jul 2013 11:24:48		
<b>Nucleus</b>	13C	<b>Number of Transients</b>	207	<b>Original Points Count</b>	16316
<b>Pulse Sequence</b>	zgpg30	<b>Solvent</b>	CHLOROFORM-D	<b>Sweep Width (Hz)</b>	18115.94
				<b>Frequency (MHz)</b>	75.48
				<b>Points Count</b>	16384
				<b>Temperature (degree C)</b>	27.200



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	Annotation	(ppm)
1	22.54	1701.5	0.2455	8	129.23	9753.7	0.1297	1	Chloroform-d	77.00
2	28.33	2138.3	0.1370	9	131.21	9903.0	0.6461			
3	29.96	2261.0	0.1456	10	164.16	12389.9	0.1883			
4	40.55	3060.5	0.2276	11	194.88	14708.7	0.1425			
5	55.54	4191.7	0.2863	12	204.24	15415.3	0.0671			
6	60.97	4601.9	0.2348	13	207.92	15692.9	0.0695			
7	114.11	8612.6	0.4498							

<sup>1</sup>H NMR of 3-(4-bromobenzoyl)heptane-2,6-dione (2g)

<b>Acquisition Time (sec)</b>	1.3518	<b>Date</b>	13 Feb 2013 10:50:40	<b>Frequency (MHz)</b>	300.13		
<b>Nucleus</b>	1H	<b>Number of Transients</b>	1	<b>Original Points Count</b>	8124	<b>Points Count</b>	8192
<b>Pulse Sequence</b>	zg	<b>Solvent</b>	CHLOROFORM-D	<b>Sweep Width (Hz)</b>	6009.62		
<b>Temperature (degree C)</b>	27.000						



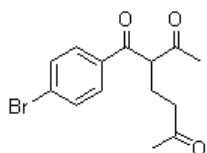
No.	Annotation	(ppm)	No.	(ppm)	Value	Absolute Value
1	Chloroform-d	7.25	1	[1.77 .. 8.45]	100.000	1.15965e+9

<sup>13</sup>C NMR of 3-(4-bromobenzoyl)heptane-2,6-dione (**2g**)

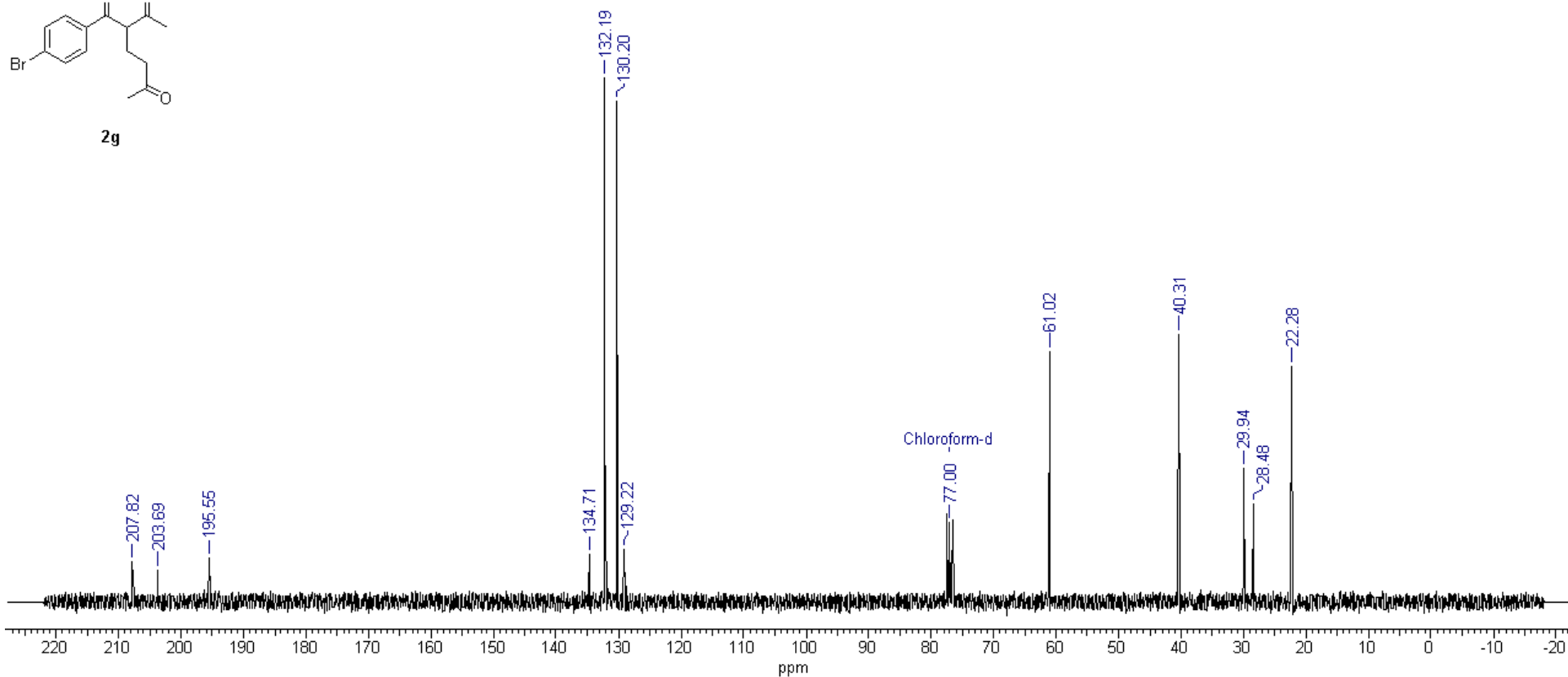
Acquisition Time (sec) 0.4501

Date 21 Sep 2013 08:49:04

Nucleus	13C	Number of Transients	173	Original Points Count	16308	Frequency (MHz)	75.48
Pulse Sequence	zpgg_baseopt	Solvent	CHLOROFORM-D	Points Count	16384	Sweep Width (Hz)	18115.94
Temperature (degree C)	22.900						



**2g**



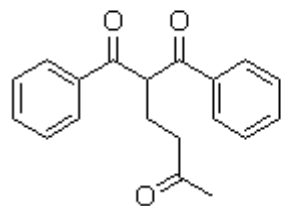
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	22.28	1681.5	0.4513	8	130.20	9826.7	0.9552
2	28.48	2149.3	0.1885	9	132.19	9977.1	1.0000
3	29.94	2259.8	0.2547	10	134.71	10167.3	0.0913
4	40.31	3042.7	0.5105	11	195.55	14759.5	0.0837
5	61.02	4605.2	0.4792	12	203.69	15373.3	0.0608
6	77.00	5811.6	0.1518	13	207.82	15685.1	0.0764
7	129.22	9752.6	0.1009				

No.	Annotation	(ppm)
1	Chloroform-d	77.00

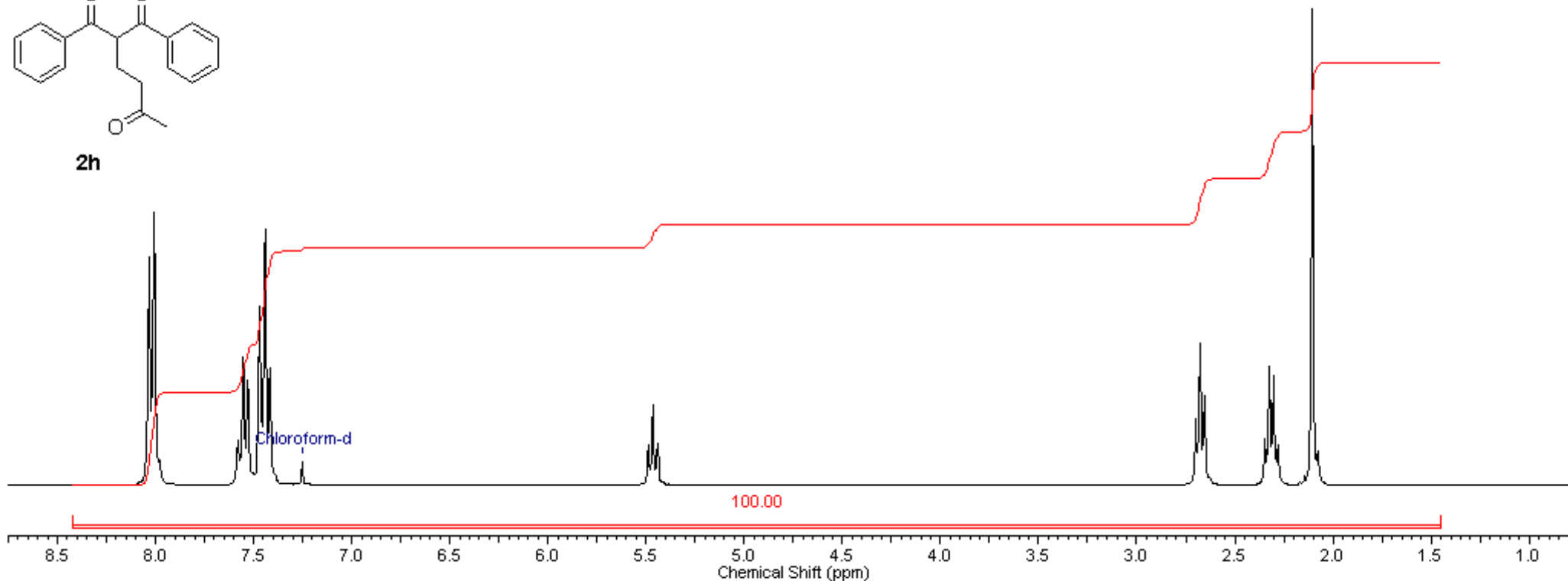


<sup>1</sup>H NMR of 2-benzoyl-1-phenylhexane-1,5-dione (**2h**)

<b>Acquisition Time (sec)</b>	1.3518	<b>Date</b>	24 Oct 2012 11:18:24		<b>Frequency (MHz)</b>	300.13	
<b>Nucleus</b>	1H	<b>Number of Transients</b>	1	<b>Original Points Count</b>	8124	<b>Points Count</b>	8192
<b>Pulse Sequence</b>	zg	<b>Solvent</b>	CHLOROFORM-D		<b>Sweep Width (Hz)</b>	6009.62	
<b>Temperature (degree C)</b>	28.800						



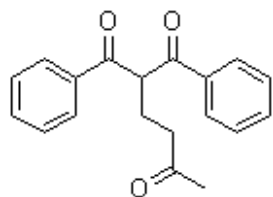
**2h**



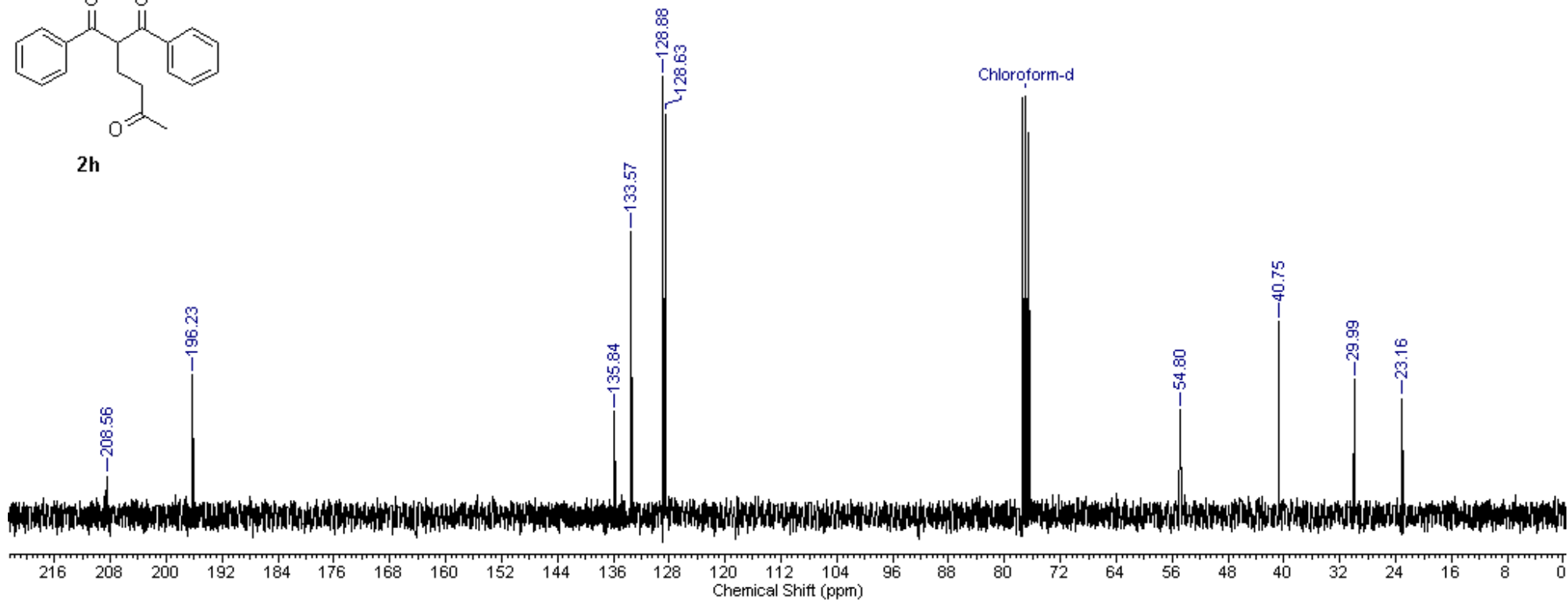
No.	Annotation	(ppm)	No.	(ppm)	Value	Absolute Value
1	Chloroform-d	7.25	1	[1.45 .. 8.42]	100.000	2.11414e+9

<sup>13</sup>C NMR of 2-benzoyl-1-phenylhexane-1,5-dione (**2h**)

<b>Acquisition Time (sec)</b>	0.9002	<b>Comment</b>	Avance-300, C-13, CDCl3		<b>Date</b>	24 Oct 2012 11:20:32	
<b>Nucleus</b>	13C	<b>Number of Transients</b>	108	<b>Original Points Count</b>	16308	<b>Frequency (MHz)</b>	75.48
<b>Pulse Sequence</b>	zgpg30base	<b>Solvent</b>	CHLOROFORM-D	<b>Sweep Width (Hz)</b>	18115.94	<b>Points Count</b>	16364
						<b>Temperature (degree C)</b>	28.900



**2h**



No.	(ppm)	(Hz)	Height
1	23.16	1747.9	0.2665
2	29.99	2263.2	0.3091
3	40.75	3076.0	0.4426
4	54.80	4136.4	0.2409
5	128.63	9708.4	0.9153
6	128.88	9727.2	1.0000
7	133.57	10081.1	0.6480
8	135.84	10252.5	0.2363
9	196.23	14810.5	0.3191
10	208.56	15741.5	0.0891

No.	Annotation	(ppm)
1	Chloroform-d	77.00

<sup>1</sup>H NMR of 3-(adamant-1-ylcarbonyl)heptane-2,6-dione (**2i**)

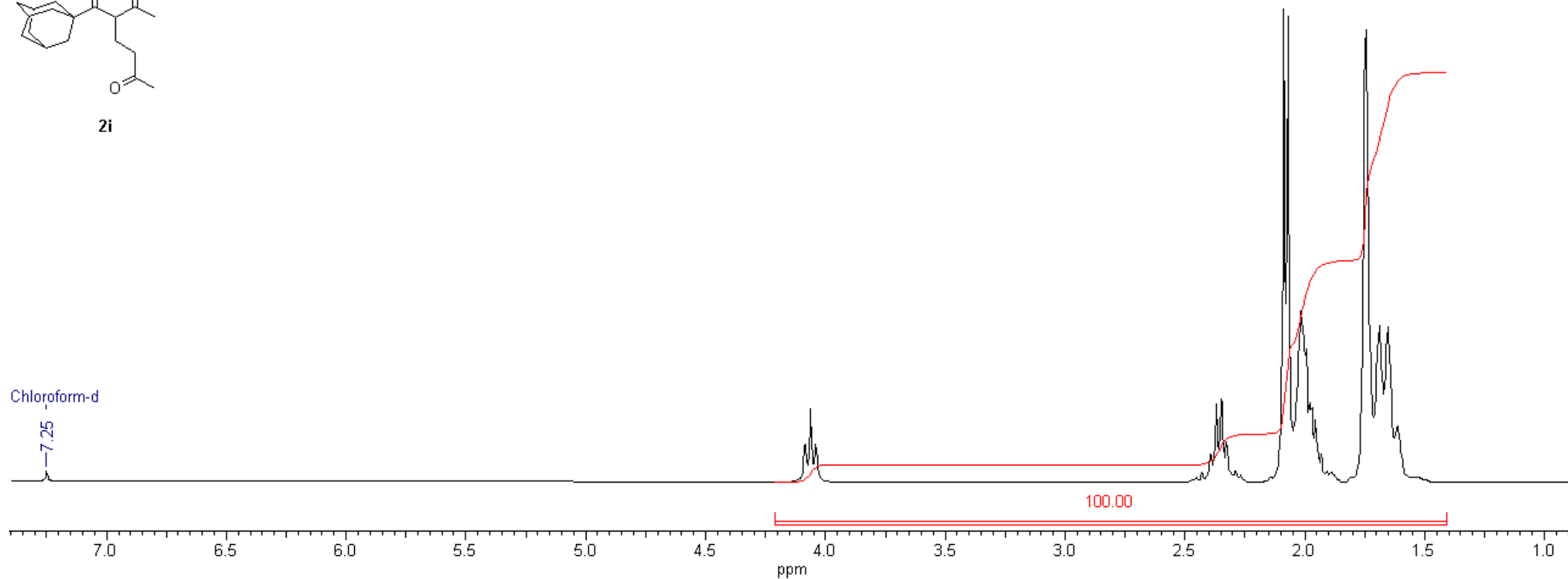
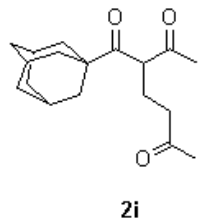
Acquisition Time (sec) 0.6759

Date 13 Nov 2012 11:48:16

Nucleus 1H  
Pulse Sequence zg  
Temperature (degree C) 27.000

Number of Transients 1  
Original Points Count 8124  
Solvent CHLOROFORM-D

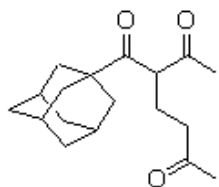
Frequency (MHz) 300.13  
Points Count 8192  
Sweep Width (Hz) 6009.62



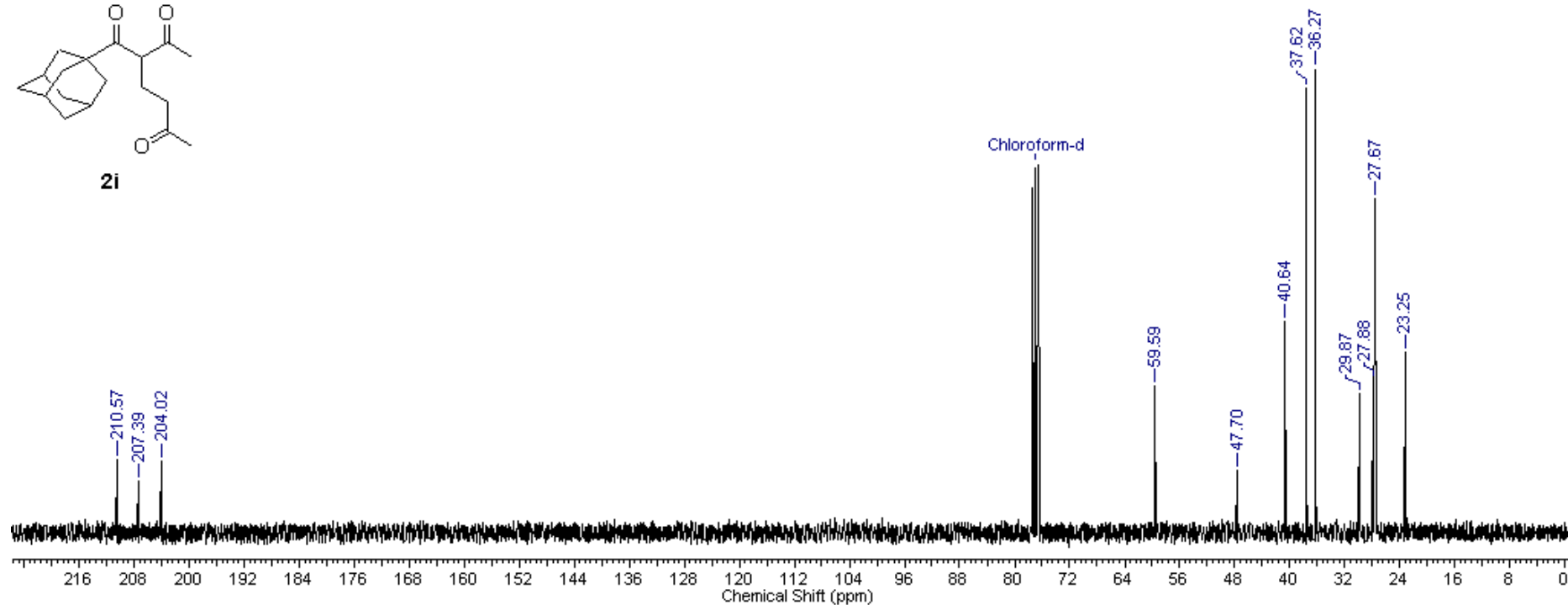
No.	(ppm)	(Hz)	Height	No.	Annotation	(ppm)	No.	(ppm)	Value
1	7.25	2176.0	0.0234	1	Chloroform-d	7.25	1	.41 .. 4.2	100.000

<sup>13</sup>C NMR of 3-(adamant-1-ylcarbonyl)heptane-2,6-dione (**2i**)

<b>Acquisition Time (sec)</b>	0.9002	<b>Comment</b>	Avance-300, C-13, CDCl3		<b>Date</b>	13 Nov 2012 11:50:24	
<b>Nucleus</b>	13C	<b>Number of Transients</b>	160	<b>Original Points Count</b>	16308	<b>Frequency (MHz)</b>	75.48
<b>Pulse Sequence</b>	zgpg30base	<b>Solvent</b>	CHLOROFORM-D	<b>Sweep Width (Hz)</b>	18115.94	<b>Points Count</b>	16384
						<b>Temperature (degree C)</b>	27.900



**2i**

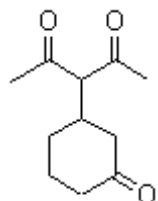


No.	(ppm)	(Hz)	Height
1	23.25	1754.6	0.3888
2	27.67	2088.5	0.7190
3	27.88	2104.0	0.3279
4	29.87	2254.4	0.3007
5	36.27	2737.6	1.0000
6	37.62	2839.3	0.9588
7	40.64	3067.1	0.4552
8	47.70	3600.1	0.1340
9	59.59	4498.0	0.3156
10	204.02	15398.7	0.1539
11	207.39	15653.1	0.1097
12	210.57	15893.0	0.1582

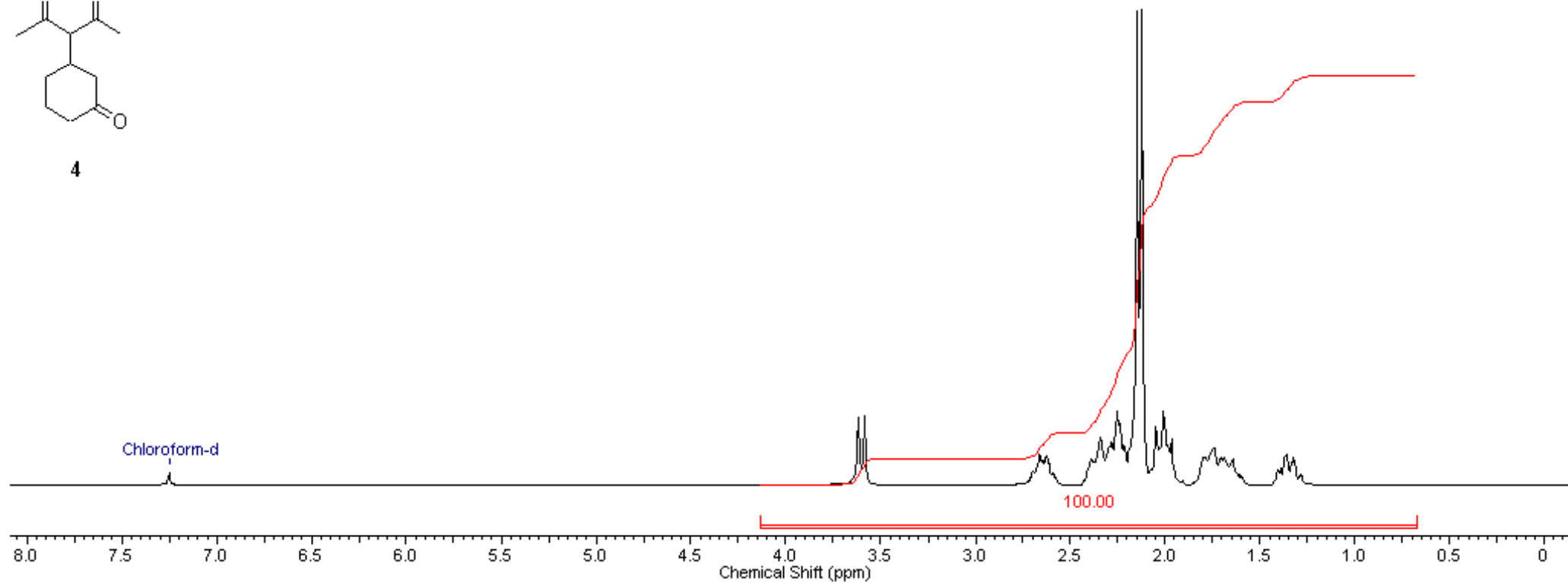
No.	Annotation	(ppm)
1	Chloroform-d	77.00

<sup>1</sup>H NMR of 3-(3-oxocyclohexyl)pentane-2,4-dione (**4**)

<b>Acquisition Time (sec)</b>	1.3518	<b>Date</b>	17 Apr 2013 15:34:24	<b>Frequency (MHz)</b>	300.13		
<b>Nucleus</b>	1H	<b>Number of Transients</b>	1	<b>Original Points Count</b>	8124	<b>Points Count</b>	8192
<b>Pulse Sequence</b>	zg31	<b>Solvent</b>	CHLOROFORM-D	<b>Sweep Width (Hz)</b>	6009.62		
<b>Temperature (degree C)</b>	28.800						



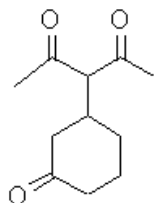
**4**



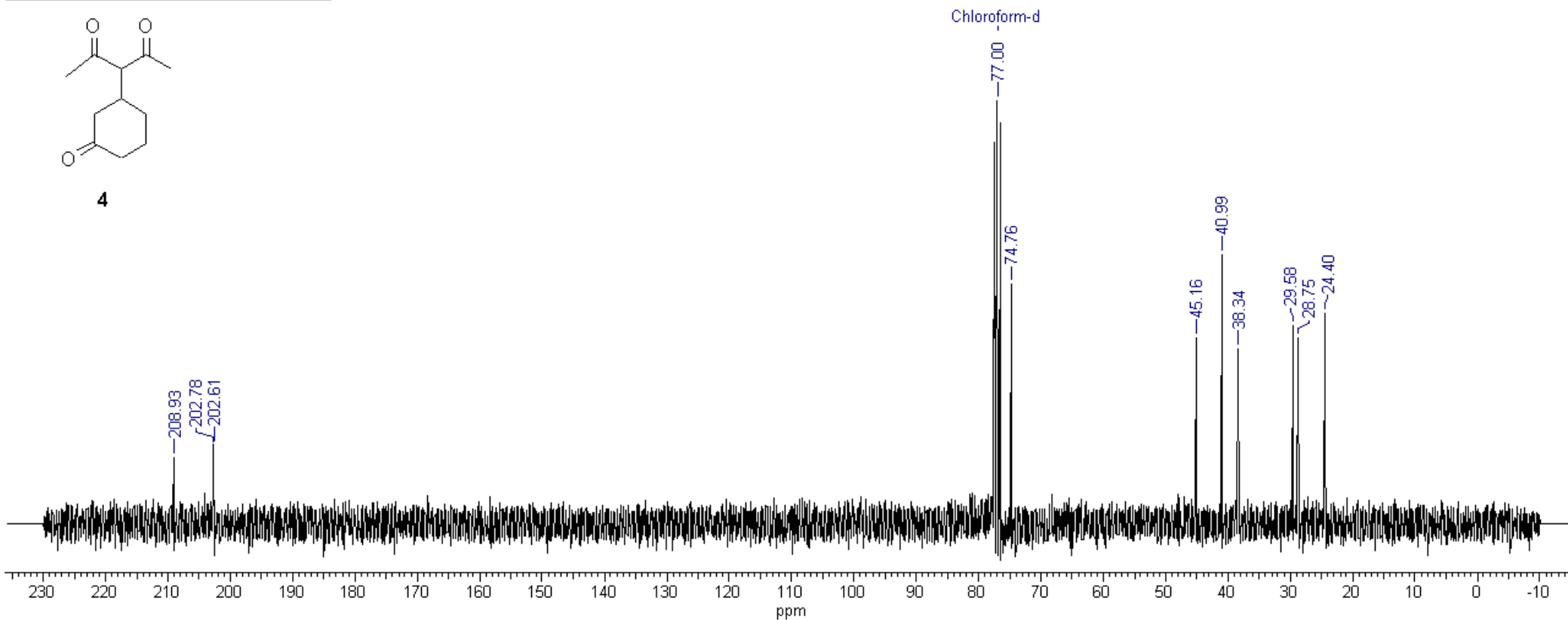
No.	Annotation	(ppm)	No.	(ppm)	Value	Absolute Value
1	Chloroform-d	7.25	1	[0.67 .. 4.13]	100.000	1.56047e+9

<sup>13</sup>C NMR of 3-(3-oxocyclohexyl)pentane-2,4-dione (**4**)

<b>Acquisition Time (sec)</b> 0.4503		<b>Date</b> 17 Apr 2013 15:34:24		
<b>Nucleus</b> 13C	<b>Number of Transients</b> 113	<b>Original Points Count</b> 16316	<b>Frequency (MHz)</b> 75.48	<b>Points Count</b> 16384
<b>Pulse Sequence</b> zgpg30	<b>Solvent</b> CHLOROFORM-D		<b>Sweep Width (Hz)</b> 18115.94	
<b>Temperature (degree C)</b> 28.800				



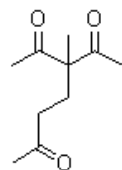
**4**



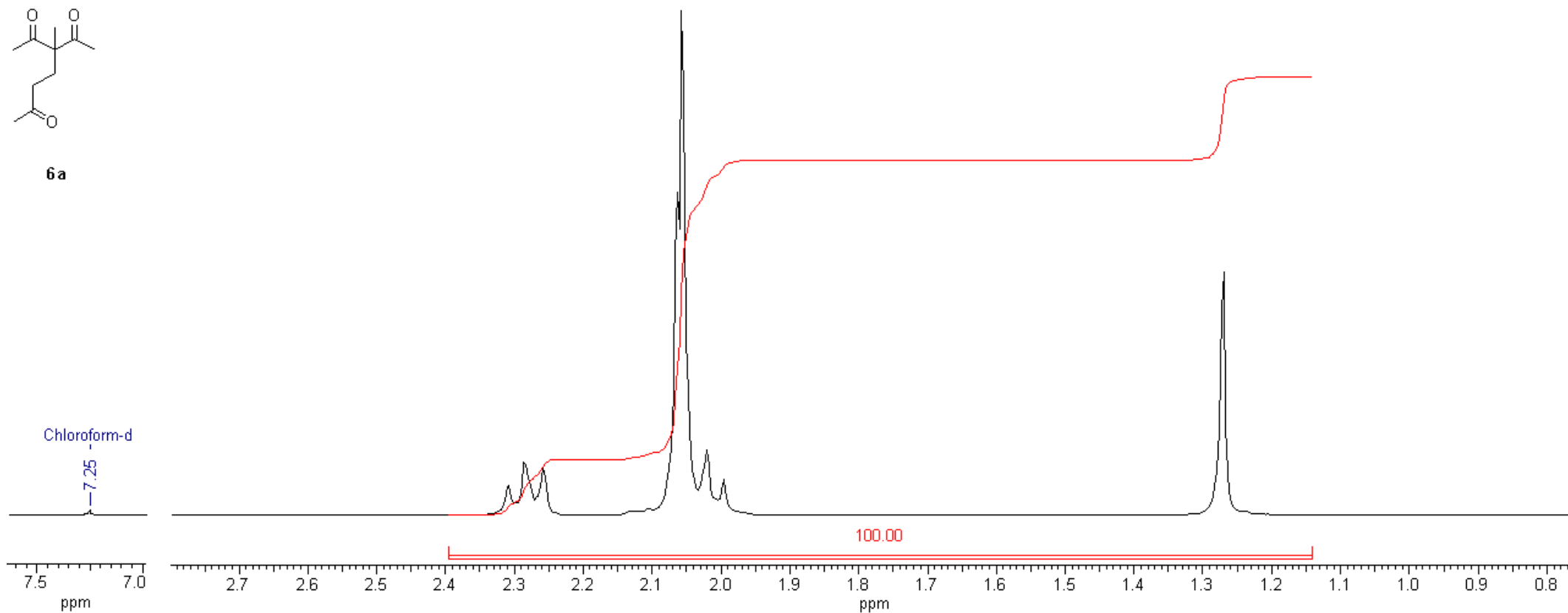
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	Annotation	(ppm)
1	24.40	1841.9	0.4971	7	45.16	3408.8	0.4394	1	Chloroform-d	77.00
2	28.75	2170.3	0.4377	8	74.76	5642.4	0.5650			
3	29.58	2232.2	0.4670	9	77.00	5811.6	1.0000			
4	29.69	2241.1	0.3897	10	202.61	15292.6	0.1872			
5	38.34	2893.5	0.4142	11	202.78	15304.7	0.1835			
6	40.99	3093.6	0.6361	12	208.93	15769.1	0.1572			

<sup>1</sup>H NMR of 3-acetyl-3-methylheptane-2,6-dione (**6a**)

<b>Acquisition Time (sec)</b>	0.5416	<b>Comment</b>	Avance-300, 1H CDCB	<b>Date</b>	21 Jun 2013 14:56:00		
<b>Nucleus</b>	1H	<b>Number of Transients</b>	1	<b>Original Points Count</b>	8124	<b>Frequency (MHz)</b>	300.13
<b>Pulse Sequence</b>	zg	<b>Solvent</b>	CHLOROFORM-D	<b>Points Count</b>	8192	<b>Sweep Width (Hz)</b>	7500.00
<b>Temperature (degree C)</b>	26.100						



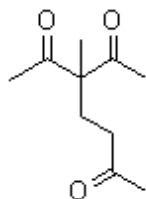
**6a**



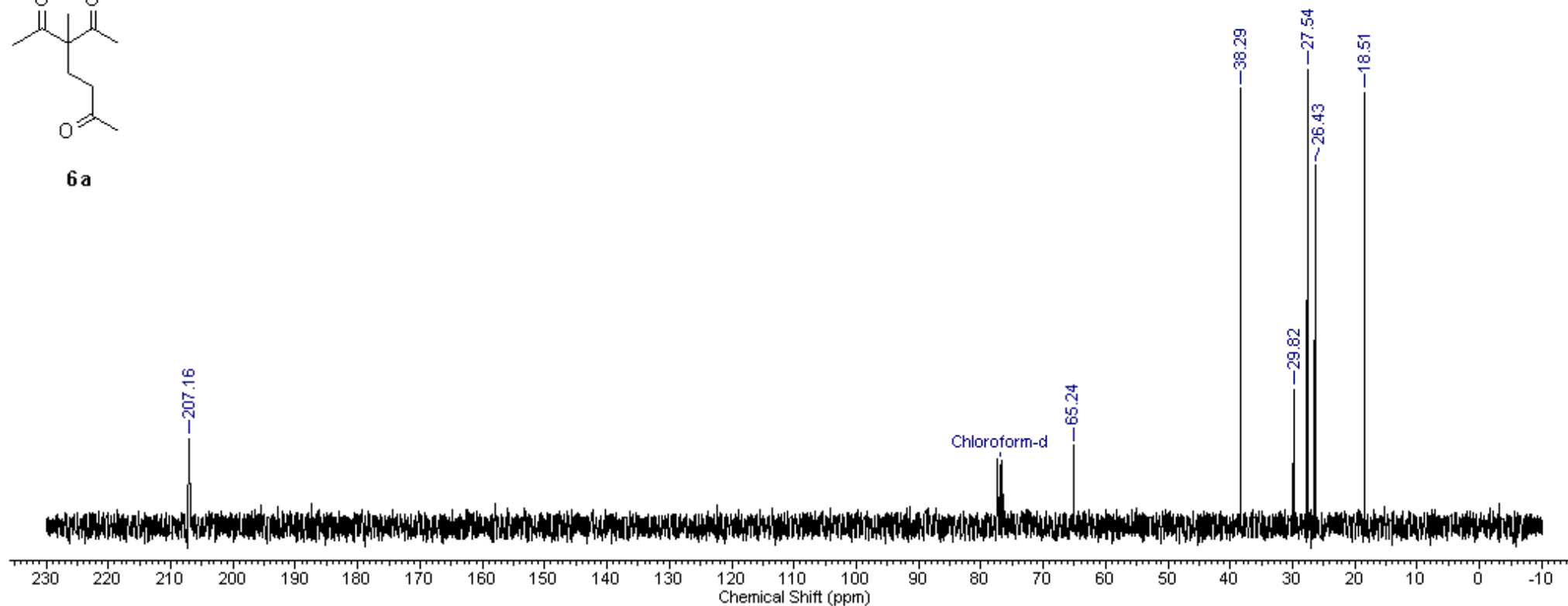
No.	(ppm)	(Hz)	Height	No.	Annotation	(ppm)	No.	(ppm)	Value
1	7.25	2175.8	0.0096	1	Chloroform-d	7.25	1	14 .. 2.4	100.000

<sup>13</sup>C NMR of 3-acetyl-3-methylheptane-2,6-dione (**6a**)

<b>Acquisition Time (sec)</b> 0.9002				<b>Date</b> 13 Jul 2013 11:52:32	
<b>File Name</b>					
<b>Nucleus</b> 13C	<b>Number of Transients</b> 58	<b>Original Points Count</b> 16308	<b>Frequency (MHz)</b> 75.48		
<b>Pulse Sequence</b> zgpg baseopt	<b>Solvent</b> CHLOROFORM-D	<b>Sweep Width (Hz)</b> 18115.94	<b>Points Count</b> 16384		
				<b>Temperature (degree C)</b> 28.000	



**6a**



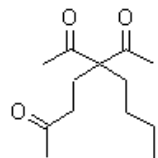
No.	(ppm)	(Hz)	Height
1	18.51	1397.4	0.9492
2	26.43	1994.5	0.7890
3	27.54	2078.6	1.0000
4	29.82	2251.1	0.2993
5	38.29	2890.2	0.9575
6	65.24	4923.7	0.1770
7	207.16	15635.4	0.1920

No.	Annotation	(ppm)
1	Chloroform-d	77.00

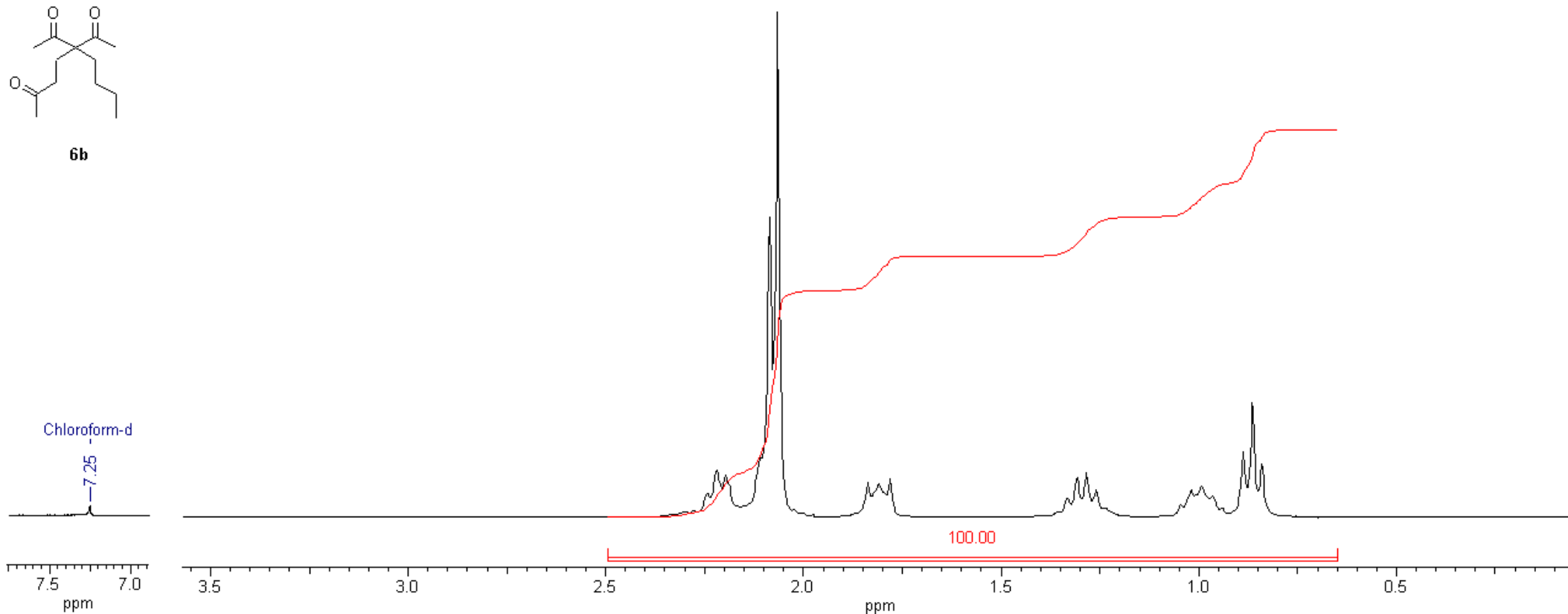


<sup>1</sup>H NMR of 3-acetyl-3-butylheptane-2,6-dione (**6b**)

<b>Acquisition Time (sec)</b> 0.6759		<b>Date</b> 24 Jun 2013 12:41:36		<b>Frequency (MHz)</b> 300.13
<b>Nucleus</b> 1H	<b>Number of Transients</b> 1	<b>Original Points Count</b> 8124	<b>Points Count</b> 8192	
<b>Pulse Sequence</b> zg	<b>Solvent</b> CHLOROFORM-D		<b>Sweep Width (Hz)</b> 6009.62	
<b>Temperature (degree C)</b> 26.500				



**6b**



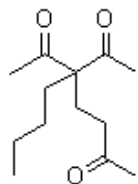
No.	(ppm)	(Hz)	Height	No.	Annotation	(ppm)	No.	(ppm)	Value
1	7.25	2176.0	0.0218	1	Chloroform-d	7.25	1	65 .. 2.4	100.000

<sup>13</sup>C NMR of 3-acetyl-3-butylheptane-2,6-dione (**6b**)

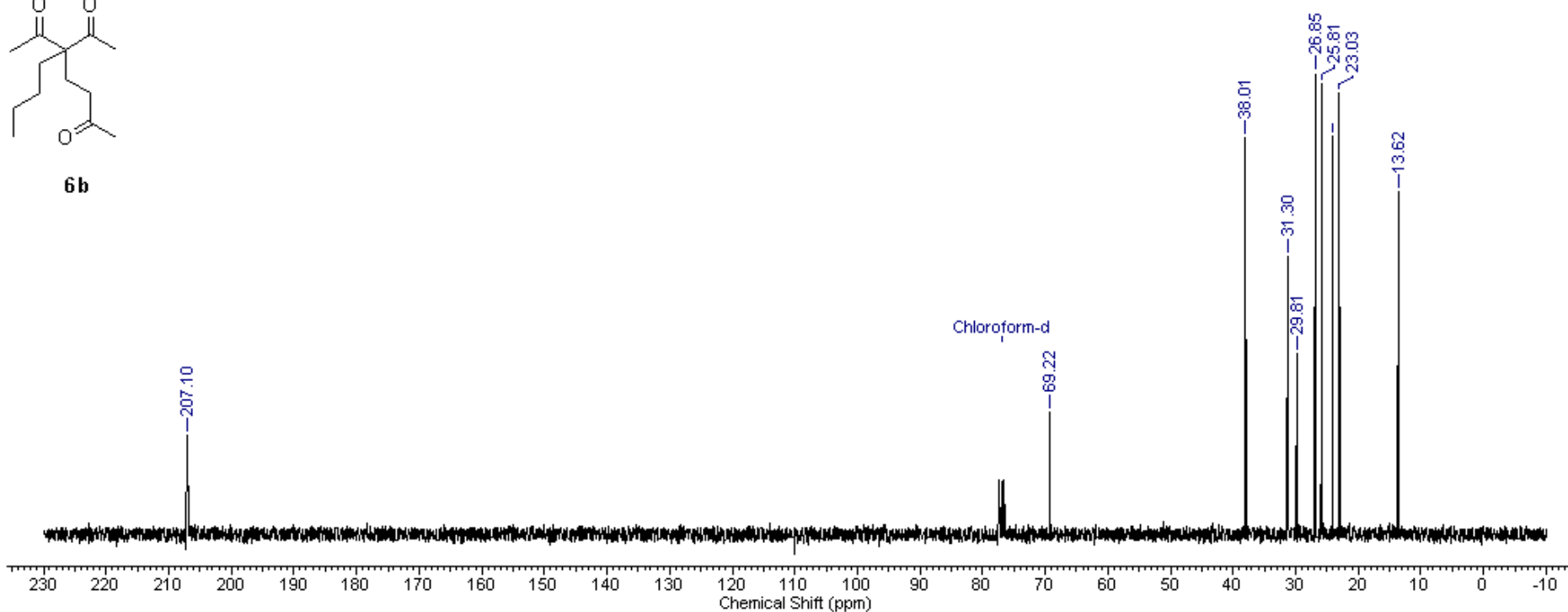
Acquisition Time (sec) 0.9002

Date 13 Jul 2013 12:01:04  
 Frequency (MHz) 75.48  
 Points Count 16384  
 Temperature (degree C) 28.200

Nucleus 13C  
 Number of Transients 121  
 Original Points Count 16308  
 Pulse Sequence zgpg\_baseopt  
 Solvent CHLOROFORM-D  
 Sweep Width (Hz) 18115.94



**6b**

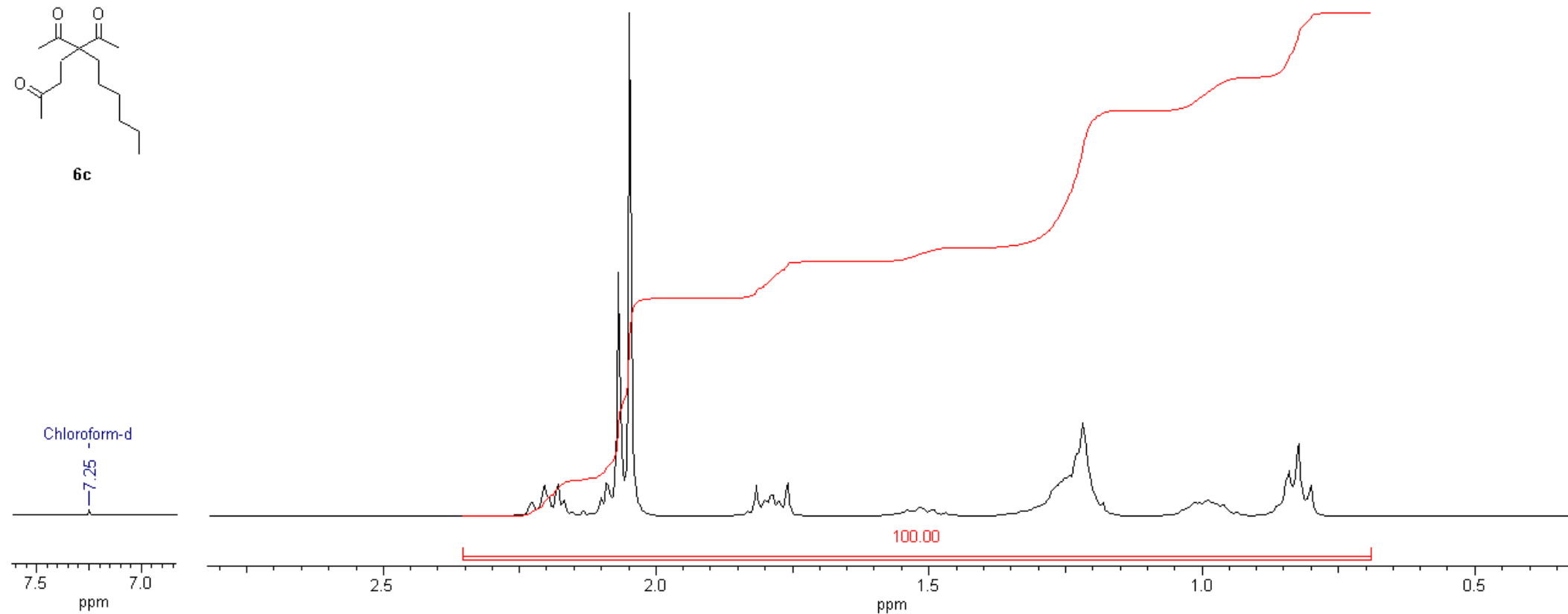
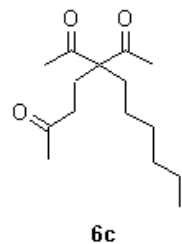


No.	(ppm)	(Hz)	Height
1	13.62	1028.1	0.7435
2	23.03	1738.0	0.9587
3	24.15	1823.1	0.8644
4	25.81	1948.1	0.9786
5	26.85	2026.6	1.0000
6	29.81	2249.9	0.3918
7	31.30	2362.7	0.6029
8	38.01	2869.2	0.8600
9	69.22	5224.5	0.2646
10	207.10	15631.0	0.2140

No.	Annotation	(ppm)
1	Chloroform-d	77.00

<sup>1</sup>H NMR of 3-acetyl-3-hexylheptane-2,6-dione (**6c**)

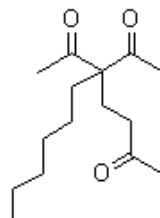
<b>Acquisition Time (sec)</b>	0.5416	<b>Comment</b>	Avance-300, 1H CDCl3		<b>Date</b>	30 Aug 2013 14:32:32		
<b>Nucleus</b>	1H	<b>Number of Transients</b>	1	<b>Original Points Count</b>	8124	<b>Frequency (MHz)</b>	300.13	
<b>Pulse Sequence</b>	zg	<b>Solvent</b>	CHLOROFORM-D		<b>Points Count</b>	8192	<b>Sweep Width (Hz)</b>	7500.00
<b>Temperature (degree C)</b>	25.500							



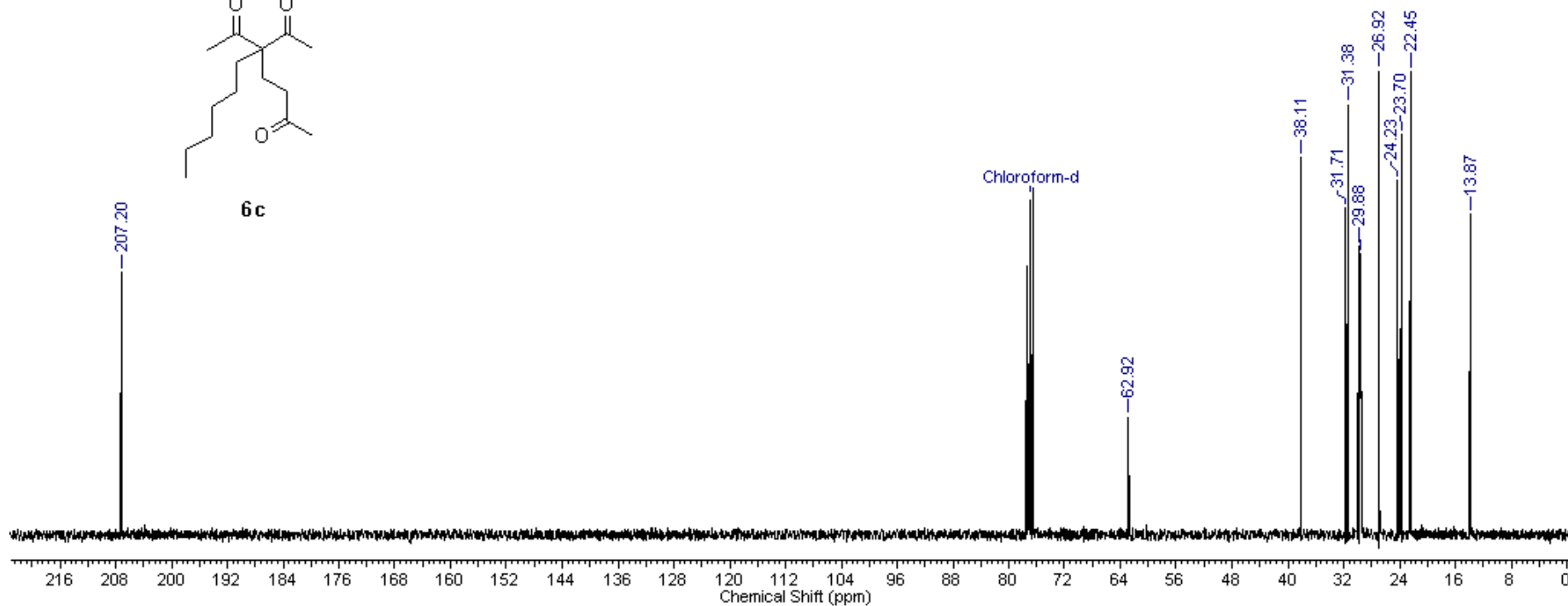
No.	(ppm)	(Hz)	Height	No.	Annotation	(ppm)	No.	(ppm)	Value
1	7.25	2175.8	0.0101	1	Chloroform-d	7.25	1	69 .. 2.3	100.000

<sup>13</sup>C NMR of 3-acetyl-3-hexylheptane-2,6-dione (**6c**)

<b>Acquisition Time (sec)</b>	0.8643	<b>Comment</b>	Avance-300, C-13, CDCl3		<b>Date</b>	30 Aug 2013 15:32:16	
<b>Nucleus</b>	13C	<b>Number of Transients</b>	548	<b>Original Points Count</b>	16308	<b>Frequency (MHz)</b>	75.48
<b>Pulse Sequence</b>	zgpg60base	<b>Solvent</b>	CHLOROFORM-D	<b>Sweep Width (Hz)</b>	18867.92	<b>Points Count</b>	16384
						<b>Temperature (degree C)</b>	26.900



**6c**

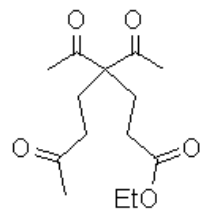


No.	(ppm)	(Hz)	Height
1	13.87	1047.1	0.6909
2	22.45	1694.4	0.9989
3	23.70	1788.8	0.8635
4	24.23	1829.1	0.7648
5	26.92	2031.8	1.0000
6	29.68	2240.3	0.6064
7	29.88	2255.2	0.6230
8	31.38	2368.1	0.9271
9	31.71	2393.4	0.7047
10	38.11	2876.0	0.8130
11	62.92	4748.6	0.2543
12	207.20	15638.9	0.5662

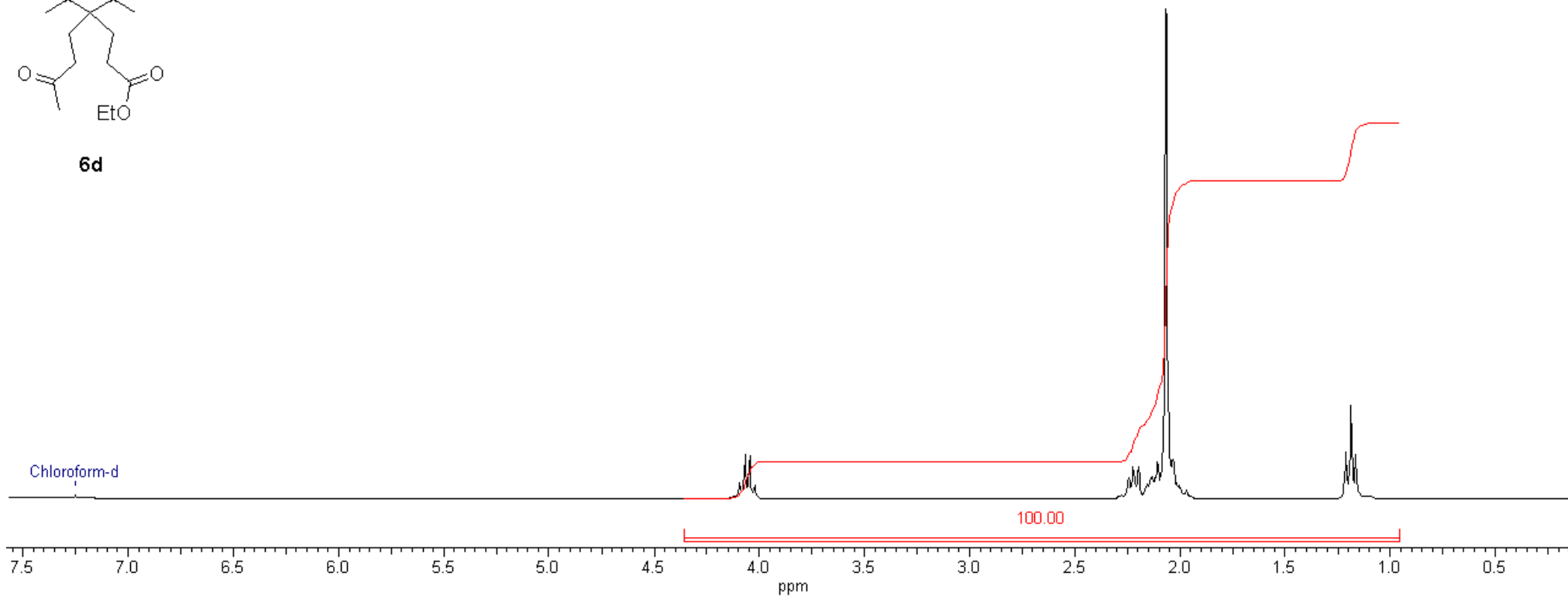
No.	Annotation	(ppm)
1	Chloroform-d	77.00

<sup>1</sup>H NMR of ethyl 4,4-diacetyl-7-oxo-octanoate (**6d**)

<b>Acquisition Time (sec)</b>	0.6759	<b>Date</b>	17 Sep 2013 10:33:36	<b>Frequency (MHz)</b>	300.13	<b>Nucleus</b>	1H
<b>Number of Transients</b>	1	<b>Original Points Count</b>	8124	<b>Points Count</b>	8192	<b>Pulse Sequence</b>	zg
<b>Solvent</b>	CHLOROFORM-D	<b>Sweep Width (Hz)</b>	6009.62	<b>Temperature (degree C)</b>	23.900		



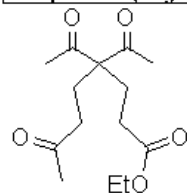
**6d**



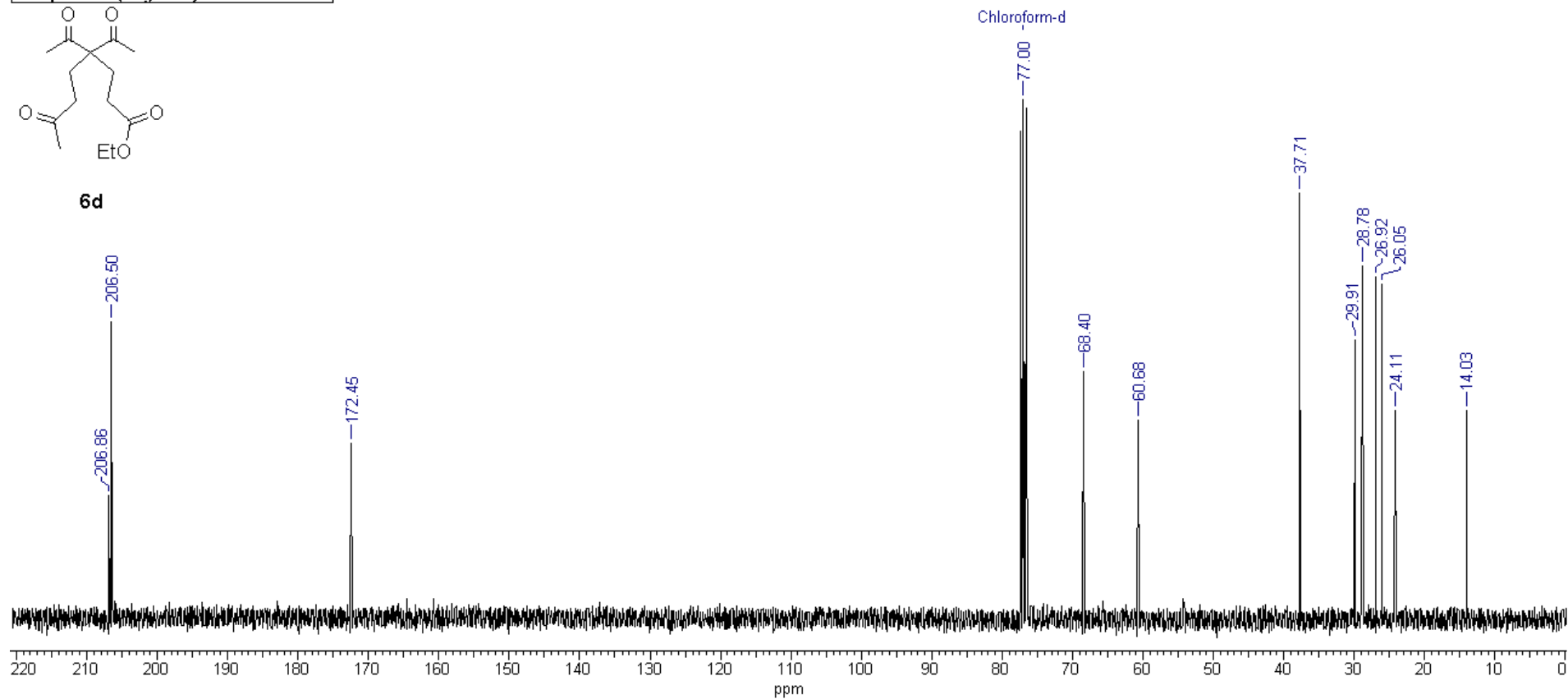
No.	Annotation	(ppm)	No.	(ppm)	Value
1	Chloroform-d	7.25	1	.96 .. 4.3	100.000

<sup>13</sup>C NMR of ethyl 4,4-diacetyl-7-oxo-octanoate (**6d**)

<b>Acquisition Time (sec)</b> 0.4503		<b>Date</b> 17 Sep 2013 14:02:40		<b>Frequency (MHz)</b> 75.48	
<b>Nucleus</b> 13C	<b>Number of Transients</b> 252	<b>Original Points Count</b> 16316	<b>Points Count</b> 16384		
<b>Pulse Sequence</b> zgpg30	<b>Solvent</b> CHLOROFORM-D		<b>Sweep Width (Hz)</b> 18115.94		
<b>Temperature (degree C)</b> 23.600					



**6d**



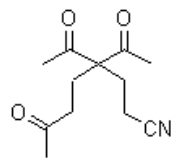
No.	(ppm)	(Hz)	Height
1	14.03	1059.0	0.4007
2	24.11	1819.8	0.4009
3	26.05	1965.8	0.6430
4	26.92	2032.1	0.6596
5	28.78	2172.6	0.6794
6	29.91	2257.7	0.5375
7	37.71	2846.0	0.8193

No.	(ppm)	(Hz)	Height
8	60.68	4579.8	0.3821
9	68.40	5162.6	0.4761
10	77.00	5811.7	1.0000
11	172.45	13015.8	0.3387
12	206.50	15585.6	0.5709
13	206.86	15613.3	0.2372

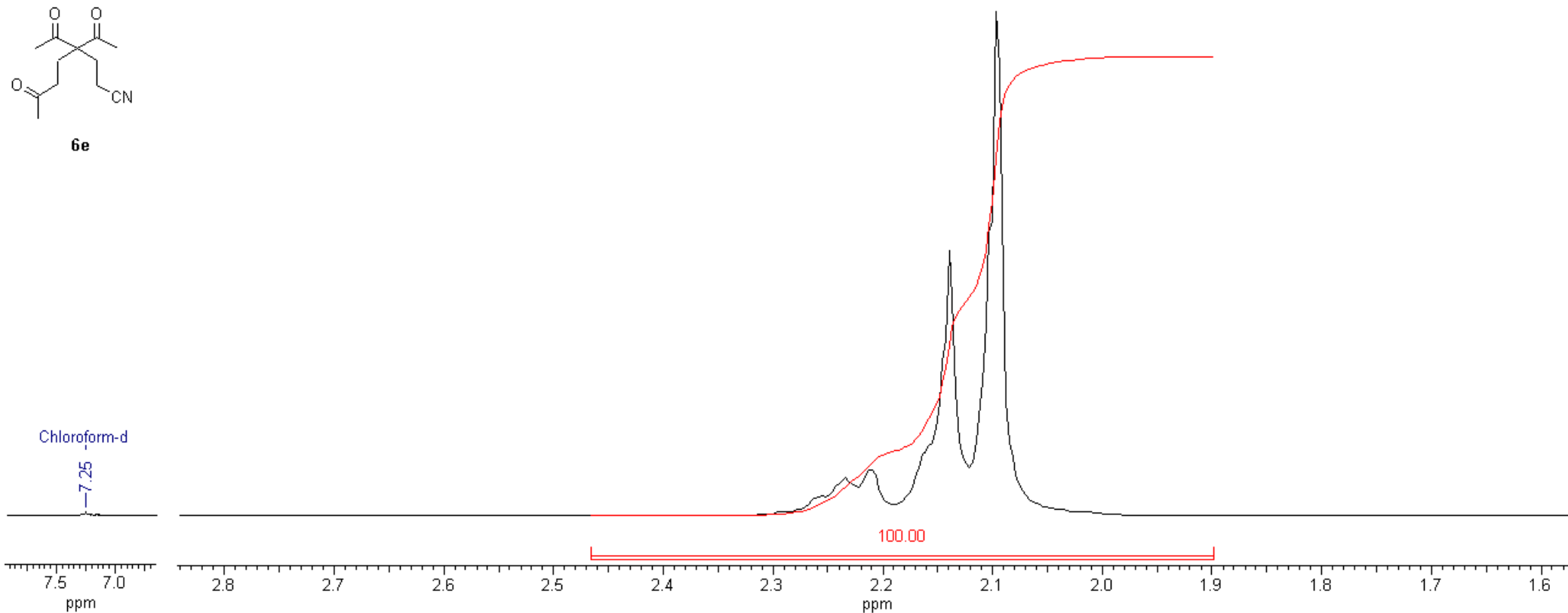
No.	Annotation	(ppm)
1	Chloroform-d	77.00

<sup>1</sup>H NMR of 4,4-diacetyl-7-oxooctanenitrile (**6e**)

<b>Acquisition Time (sec)</b>	0.5416	<b>Comment</b>	Avance-300, 1H CDCl <sub>3</sub>	<b>Date</b>	02 Aug 2013 14:51:44		
<b>Nucleus</b>	1H	<b>Number of Transients</b>	1	<b>Original Points Count</b>	8124	<b>Frequency (MHz)</b>	300.13
<b>Pulse Sequence</b>	zg	<b>Solvent</b>	CHLOROFORM-D	<b>Points Count</b>	8192	<b>Sweep Width (Hz)</b>	7500.00
<b>Temperature (degree C)</b>	25.900						



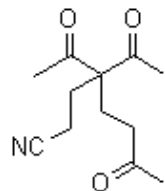
**6e**



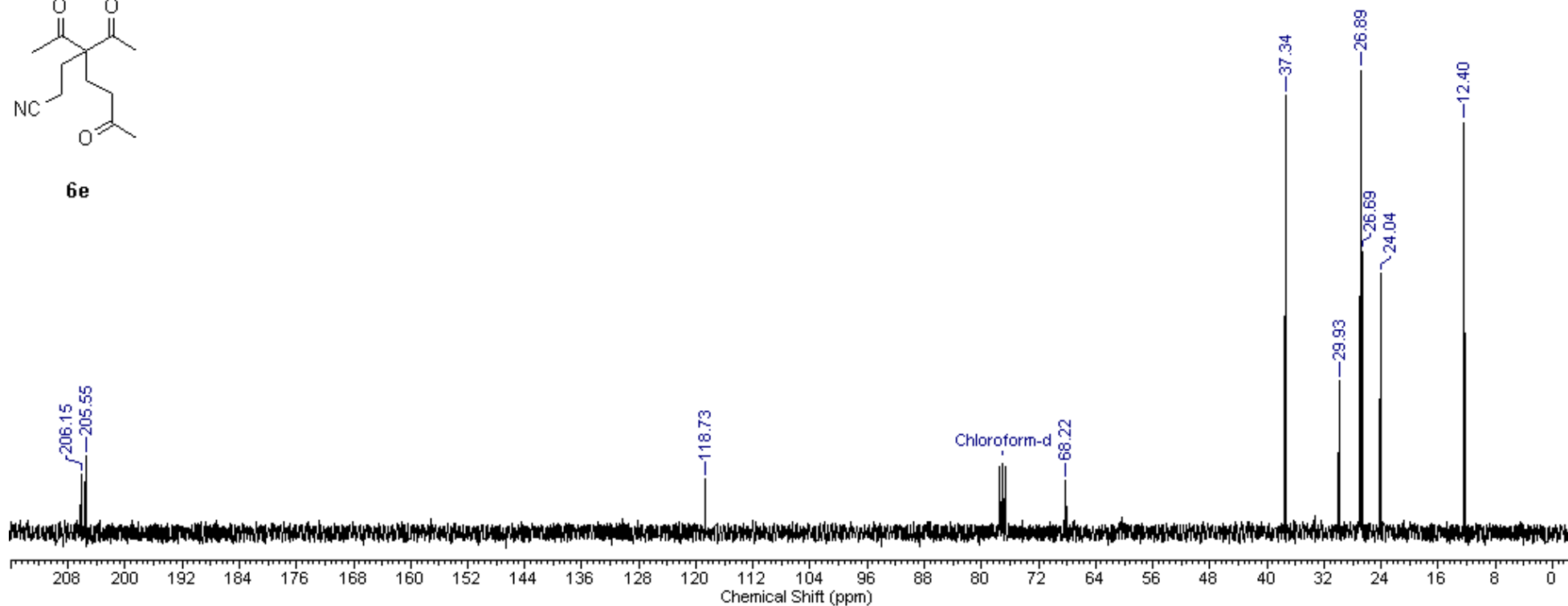
No.	(ppm)	(Hz)	Height	No.	Annotation	(ppm)	No.	(ppm)	Value
1	7.25	2175.8	0.0075	1	Chloroform-d	7.25	1	.90 .. 2.4	100.000

<sup>13</sup>C NMR of 4,4-diacetyl-7-oxooctanenitrile (**6e**)

<b>Acquisition Time (sec)</b> 0.9002				<b>Date</b> 05 Aug 2013 08:06:24	
<b>Nucleus</b> 13C	<b>Number of Transients</b> 190	<b>Original Points Count</b> 16308	<b>Frequency (MHz)</b> 75.48	<b>Points Count</b> 16384	
<b>Pulse Sequence</b> zgpg baseopt	<b>Solvent</b> CHLOROFORM-D	<b>Sweep Width (Hz)</b> 18115.94	<b>Temperature (degree C)</b> 26.600		



**6e**



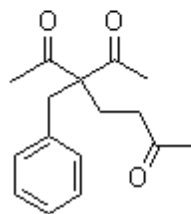
No.	(ppm)	(Hz)	Height
1	12.40	936.2	0.8870
2	24.04	1814.2	0.5612
3	26.69	2014.4	0.6084
4	26.89	2029.9	1.0000
5	29.93	2258.7	0.3295
6	37.34	2818.3	0.9466
7	68.22	5149.2	0.1124
8	118.73	8960.9	0.1146
9	205.55	15513.7	0.1667
10	206.15	15559.0	0.1263

No.	Annotation	(ppm)
1	Chloroform-d	77.00

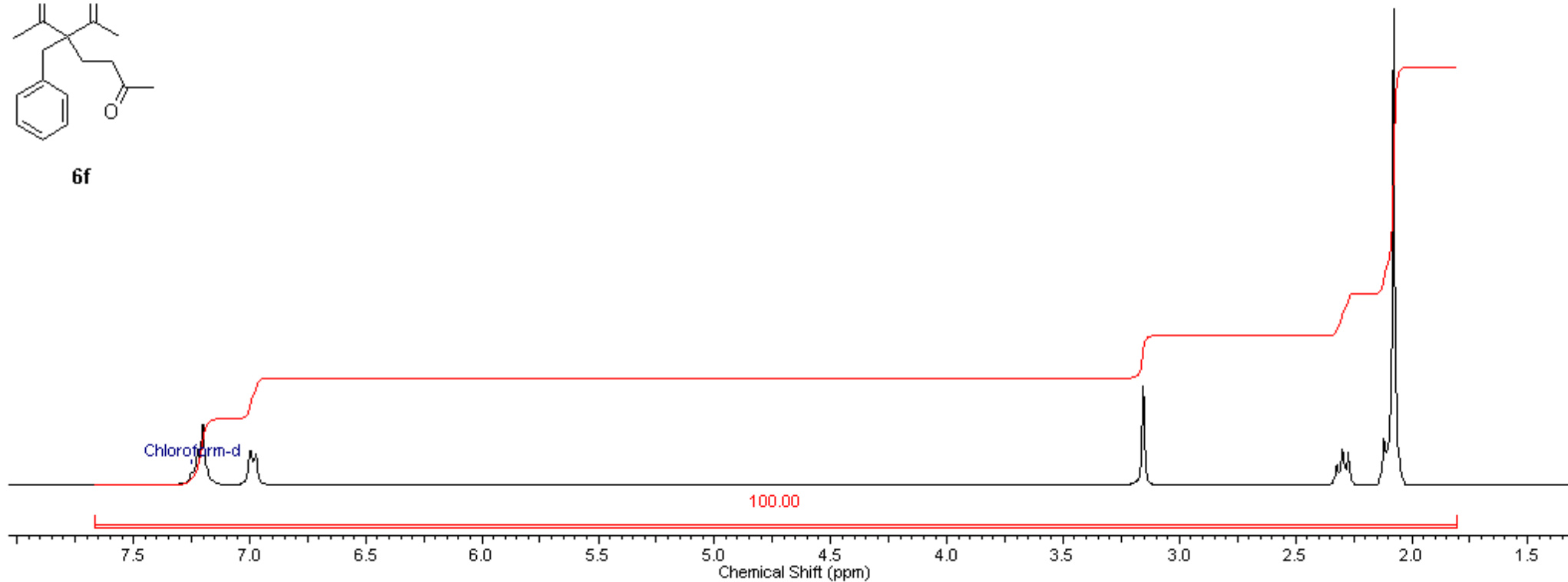


<sup>1</sup>H NMR of 3-acetyl-3-benzylpentane-2,4-dione (**6f**)

<b>Acquisition Time (sec)</b>	1.3518	<b>Date</b>	23 Jul 2013 13:37:04	<b>Frequency (MHz)</b>	300.13		
<b>Nucleus</b>	1H	<b>Number of Transients</b>	1	<b>Original Points Count</b>	8124	<b>Points Count</b>	8192
<b>Pulse Sequence</b>	zg31	<b>Solvent</b>	CHLOROFORM-D	<b>Sweep Width (Hz)</b>	6009.62		
<b>Temperature (degree C)</b>	26.700						



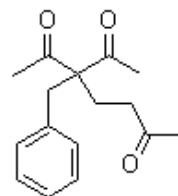
**6f**



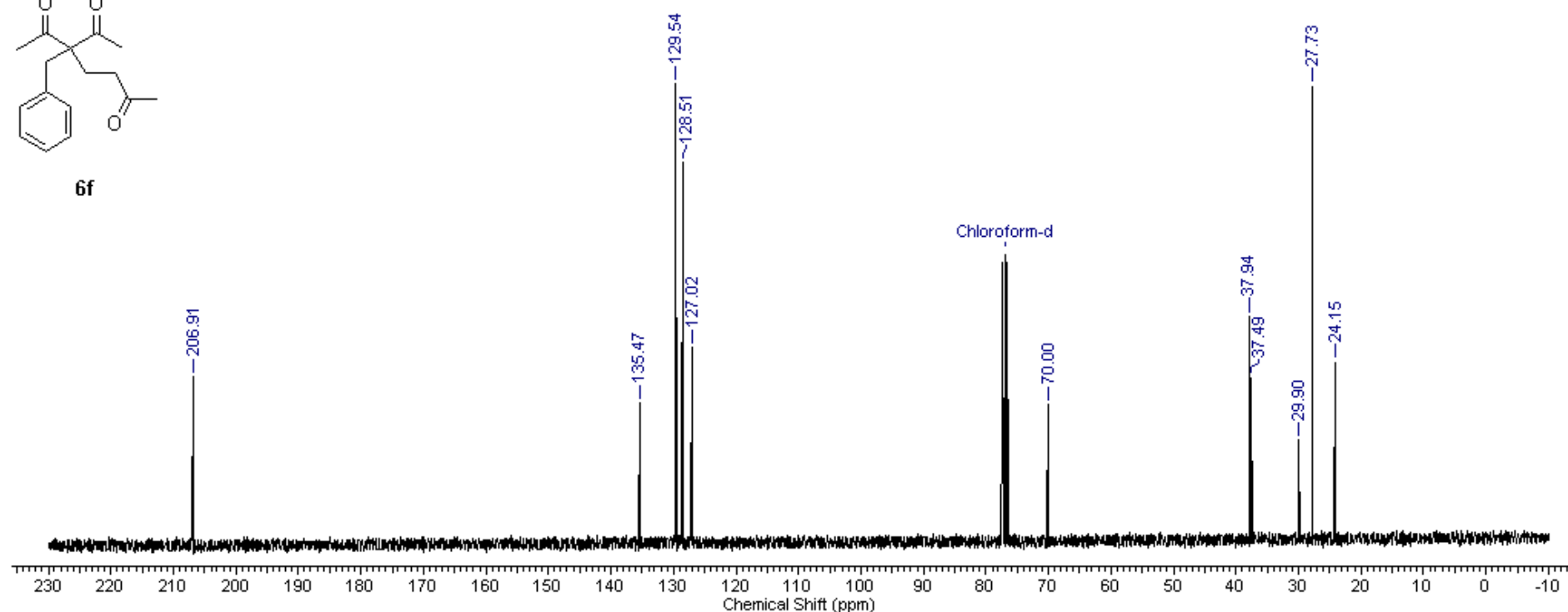
No.	Annotation	(ppm)	No.	(ppm)	Value	Absolute Value
1	Chloroform-d	7.25	1	[1.81 .. 7.67]	100.000	1.45941e+9

<sup>13</sup>C NMR of 3-acetyl-3-benzylpentane-2,4-dione (**6f**)

<b>Acquisition Time (sec)</b>	0.9006	<b>Date</b>	23 Jul 2013 13:39:12		
<b>Nucleus</b>	13C	<b>Number of Transients</b>	384	<b>Original Points Count</b>	16316
<b>Pulse Sequence</b>	zgpg30	<b>Solvent</b>	CHLOROFORM-D	<b>Sweep Width (Hz)</b>	18115.94
				<b>Frequency (MHz)</b>	75.48
				<b>Points Count</b>	16384
				<b>Temperature (degree C)</b>	26.700



**6f**

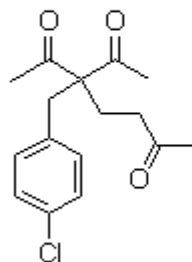


No.	(ppm)	(Hz)	Height
1	24.15	1823.1	0.3706
2	27.73	2092.9	0.9950
3	29.90	2256.6	0.1937
4	37.49	2829.4	0.3370
5	37.94	2863.7	0.4746
6	70.00	5283.1	0.2755
7	127.02	9586.8	0.4048
8	128.51	9699.6	0.8215
9	129.54	9777.0	1.0000
10	135.47	10224.8	0.2781
11	206.91	15616.6	0.3375

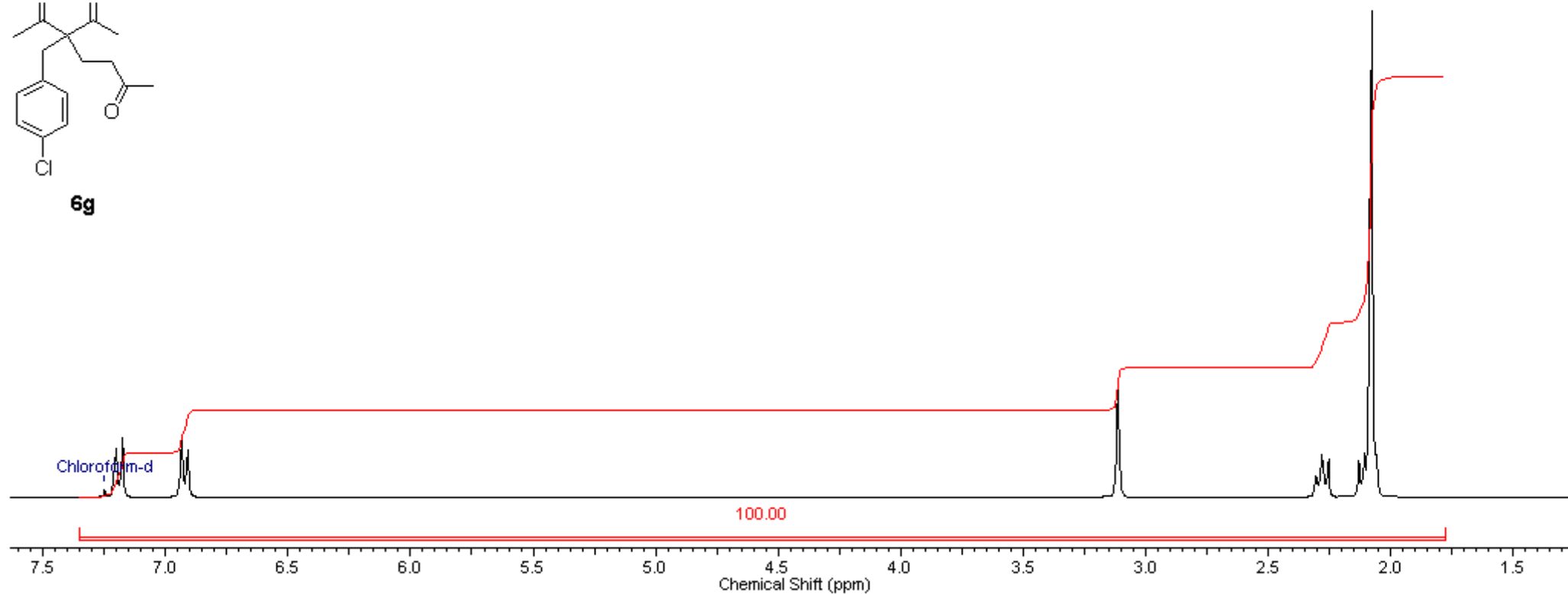
No.	Annotation	(ppm)
1	Chloroform-d	77.00

<sup>1</sup>H NMR of 3-acetyl-3-[(4-chlorophenyl)methyl]heptane-2,6-dione (**6g**)

<b>Acquisition Time (sec)</b>	1.0832	<b>Comment</b>	Avance-300, 1H CDCl3		<b>Date</b>	13 Jul 2013 13:00:48	
<b>Nucleus</b>	1H	<b>Number of Transients</b>	1	<b>Original Points Count</b>	8124	<b>Frequency (MHz)</b>	300.13
<b>Pulse Sequence</b>	zg	<b>Solvent</b>	CHLOROFORM-D	<b>Sweep Width (Hz)</b>	7500.00	<b>Points Count</b>	8192
						<b>Temperature (degree C)</b>	27.600



**6g**



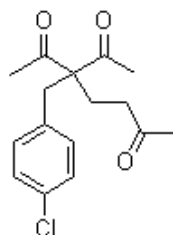
No.	Annotation	(ppm)	No.	(ppm)	Value	Absolute Value
1	Chloroform-d	7.25	1	[1.78 .. 7.35]	100.000	1.11174e+9

<sup>13</sup>C NMR of 3-acetyl-3-[(4-chlorophenyl)methyl]heptane-2,6-dione (**6g**)

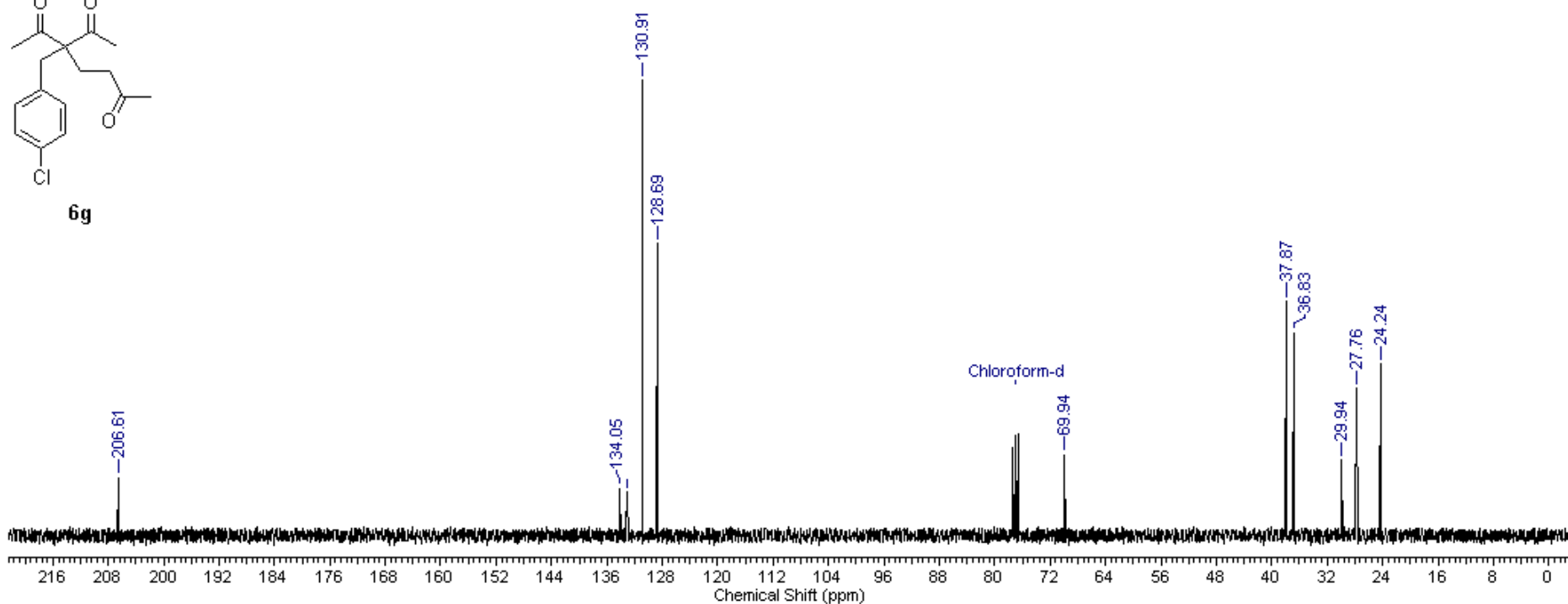
Acquisition Time (sec) 0.9002

Date 13 Jul 2013 13:11:28  
 Frequency (MHz) 75.48  
 Points Count 16384  
 Temperature (degree C) 28.100

Nucleus 13C  
 Pulse Sequence zgpg baseoct  
 Number of Transients 111  
 Solvent DMSO-D6  
 Original Points Count 16308  
 Sweep Width (Hz) 18115.94



**6g**

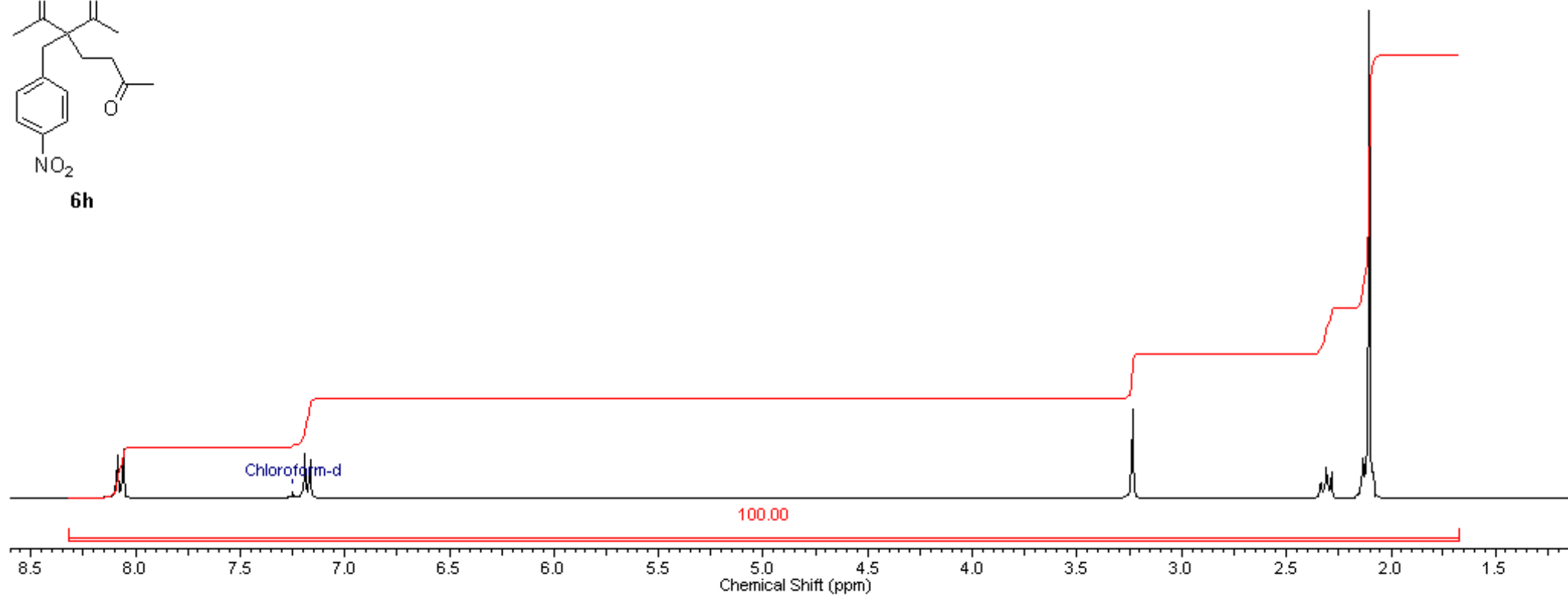
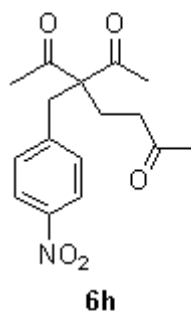


No.	(ppm)	(Hz)	Height
1	24.24	1829.8	0.3762
2	27.76	2095.1	0.3228
3	29.94	2259.9	0.1651
4	36.83	2779.6	0.4463
5	37.87	2858.1	0.5152
6	69.94	5278.7	0.1782
7	128.69	9712.8	0.6410
8	130.91	9880.9	1.0000
9	133.04	10041.3	0.0951
10	134.05	10117.6	0.1040
11	206.61	15594.5	0.1282

No.	Annotation	(ppm)
1	Chloroform-d	77.00

<sup>1</sup>H NMR of 3-acetyl-3-[(4-nitrophenyl)methyl]heptane-2,6-dione (**6h**)

<b>Acquisition Time (sec)</b>	1.0832	<b>Comment</b>	Avance-300, 1H CDCl3		<b>Date</b>	30 Aug 2013 09:25:20	
<b>Nucleus</b>	1H	<b>Number of Transients</b>	1	<b>Original Points Count</b>	8124	<b>Frequency (MHz)</b>	300.13
<b>Pulse Sequence</b>	zgq	<b>Solvent</b>	CHLOROFORM-D	<b>Sweep Width (Hz)</b>	7500.00	<b>Points Count</b>	8192
						<b>Temperature (degree C)</b>	25.800



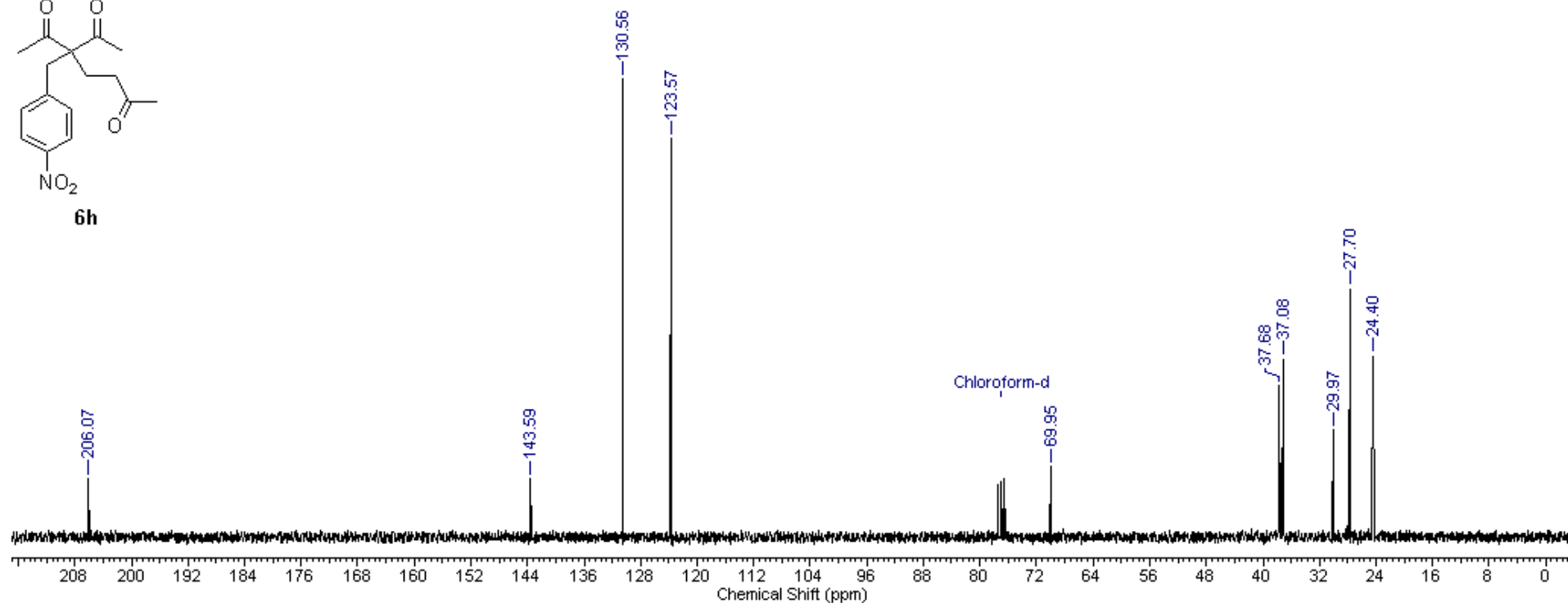
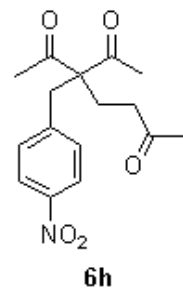
No.	Annotation	(ppm)	No.	(ppm)	Value	Absolute Value
1	Chloroform-d	7.25	1	[1.68 .. 8.32]	100.000	1.29310e+9

<sup>13</sup>C NMR of 3-acetyl-3-[(4-nitrophenyl)methyl]heptane-2,6-dione (**6h**)

Acquisition Time (sec) 0.9002

Date 30 Aug 2013 09:31:44  
 Frequency (MHz) 75.48  
 Points Count 16384  
 Temperature (degree C) 26.200

Nucleus	13C	Number of Transients	183	Original Points Count	16308
Pulse Sequence	zgpg baseopt	Solvent	CHLOROFORM-D	Sweep Width (Hz)	18115.94



No.	(ppm)	(Hz)	Height
1	24.40	1841.9	0.3948
2	27.70	2090.7	0.5423
3	29.97	2262.1	0.2325
4	37.08	2798.4	0.3890
5	37.68	2843.7	0.3301
6	69.95	5279.7	0.1538
7	123.57	9326.9	0.8700
8	130.56	9854.3	1.0000
9	143.59	10837.4	0.1274
10	206.07	15553.5	0.1288

No.	Annotation	(ppm)
1	Chloroform-d	77.00

## HRMS of 5-acetyl-8-methylnonane-2,6-dione (**2b**)

### Display Report

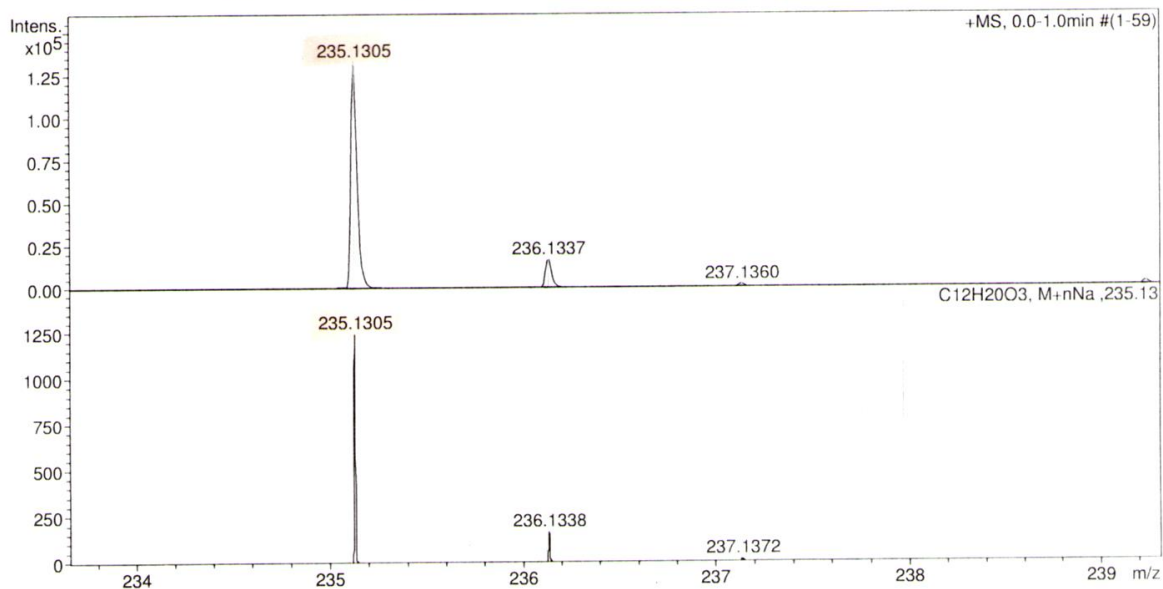
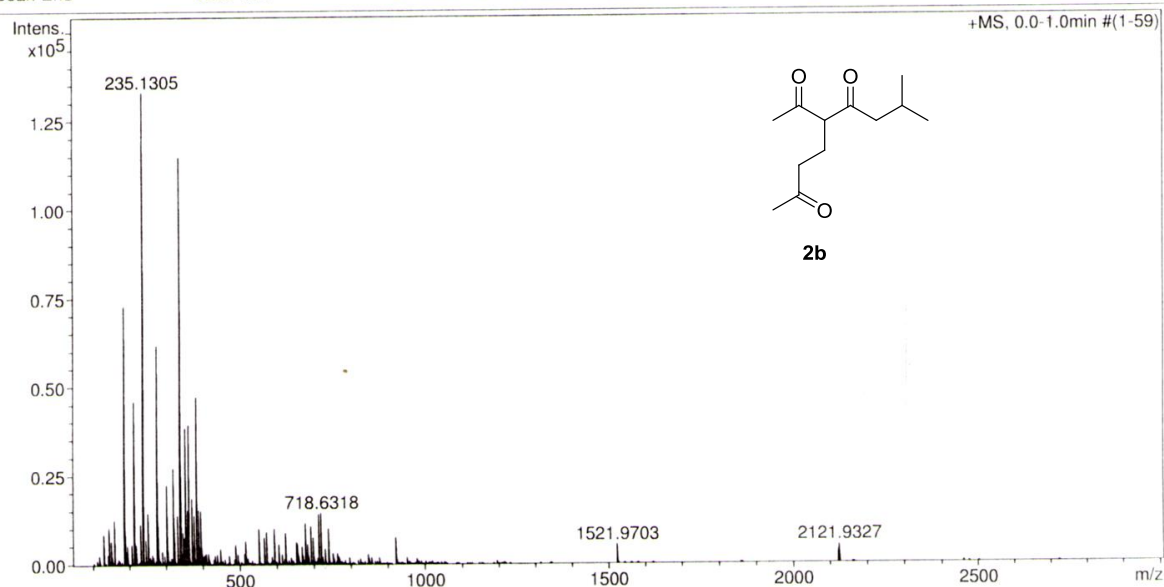
#### Analysis Info

Analysis Name D:\Data\Chizhov\Nikishin\Terentiev\Wil\bb-345\_&clblow.d  
Method tune\_low.m  
Sample Name /TERN BB-345  
Comment CH3CN 100 %, dil. 200, calibrant added

Acquisition Date 04-Mar-13 11:41:59  
Operator BDAL@DE  
Instrument / Ser# micrOTOF 10248

#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



## HRMS of 8-methyl-5-propionylnonane-2,6-dione (2c)

### Display Report

#### Analysis Info

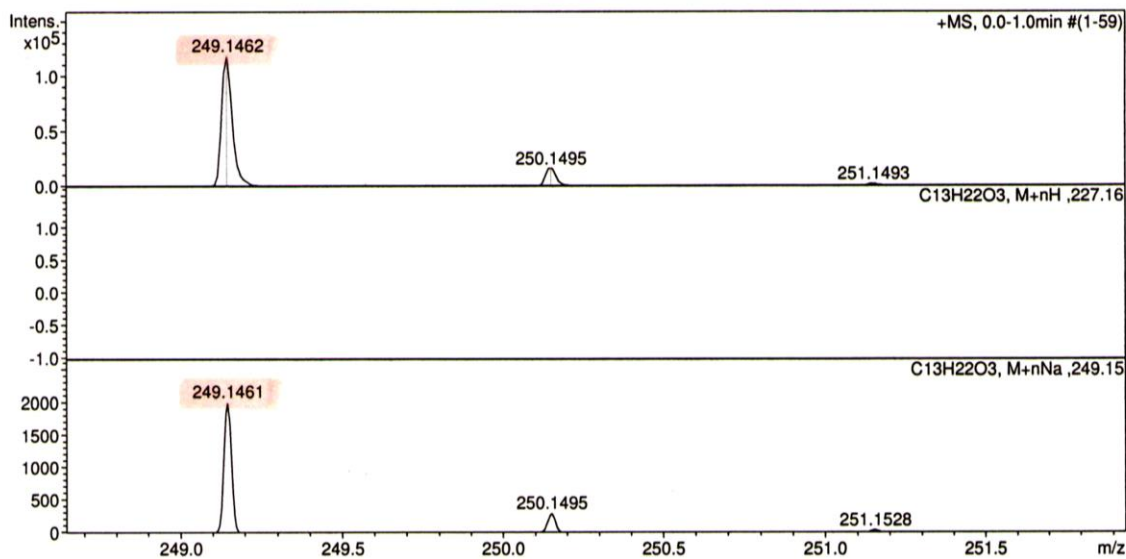
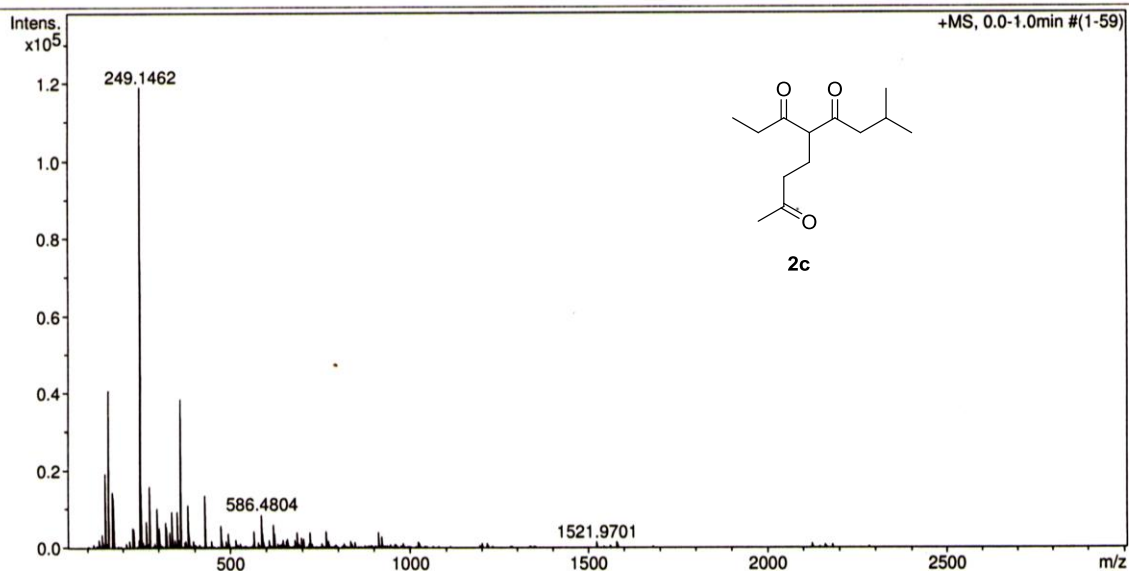
Analysis Name D:\Data\Chizhov\Nikishin\Terentiev\Wil\bb-348\_\&clblow.d  
Method tune\_low.m  
Sample Name /TERN BB-348  
Comment CH3CN 100 %, dil. > 2000, calibrant added

Acquisition Date 07.04.2013 12:46:09

Operator BDAL@DE  
Instrument / Ser# micrOTOF 10248

#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





### HRMS of 3-(adamant-1-ylcarbonyl)heptane-2,6-dione (2i)

## Display Report

#### Analysis Info

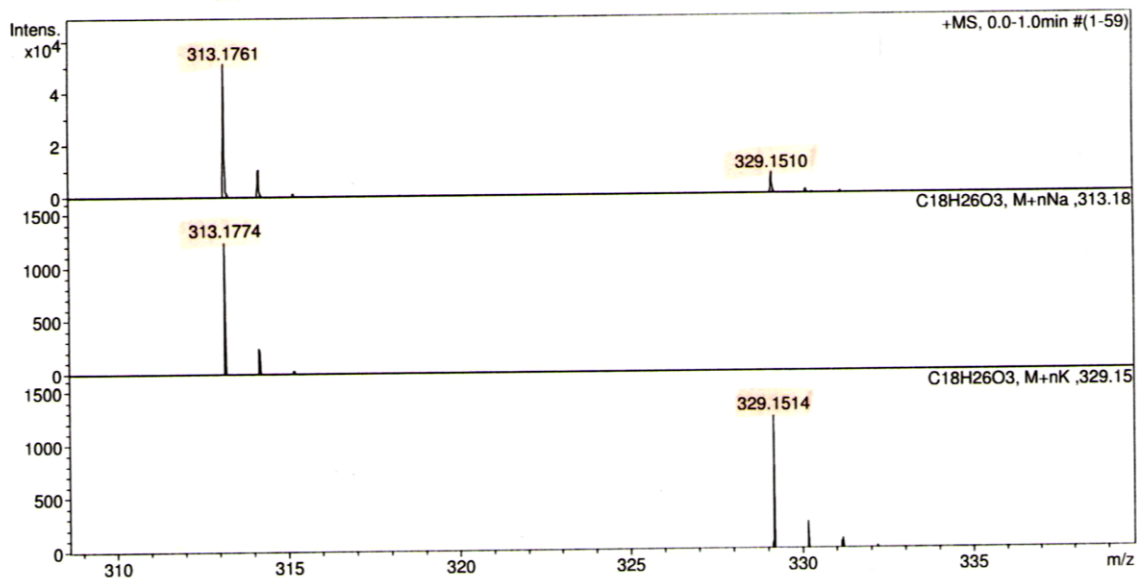
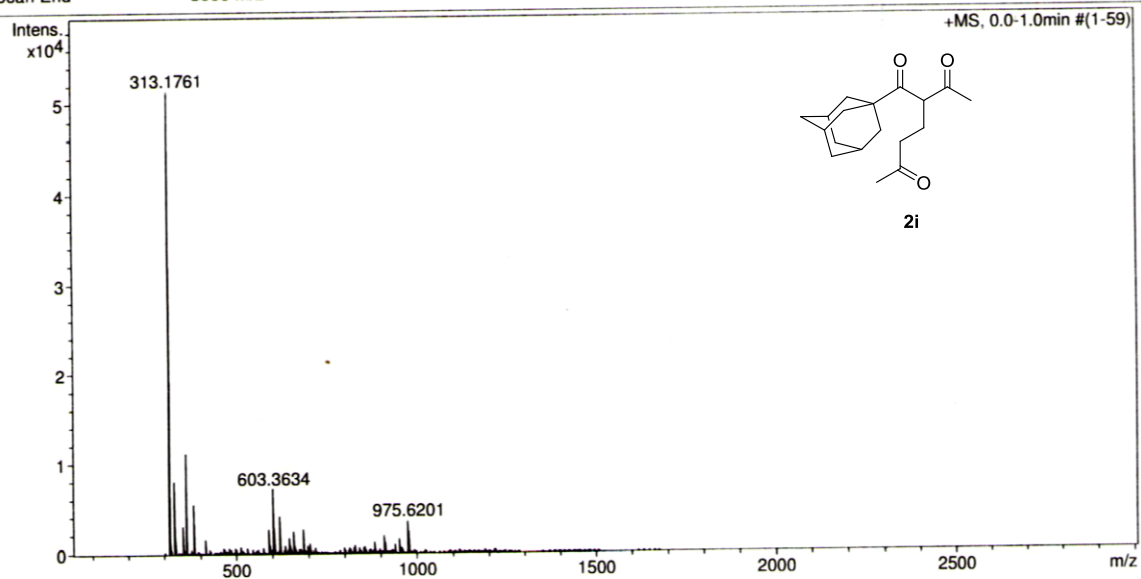
Analysis Name D:\Data\Chizhov\Nikishin\Terentiev\Wilbb291\_d  
Method tune\_wide.m  
Sample Name /TERN BB-291  
Comment CH3CN 100%, dil. 200, no calibrant added

Acquisition Date 23-Feb-13 13:08:02

Operator BDAL@DE  
Instrument / Ser# micrOTOF 10248

#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



## HRMS of 3-acetyl-3-hexylheptane-2,6-dione (**6c**)

### Display Report

#### Analysis Info

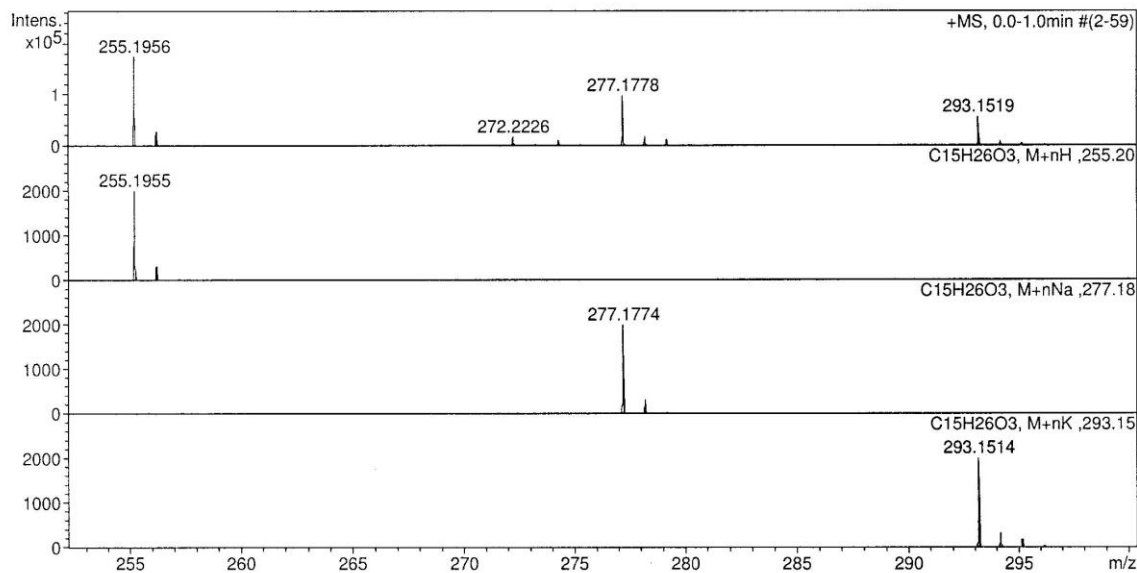
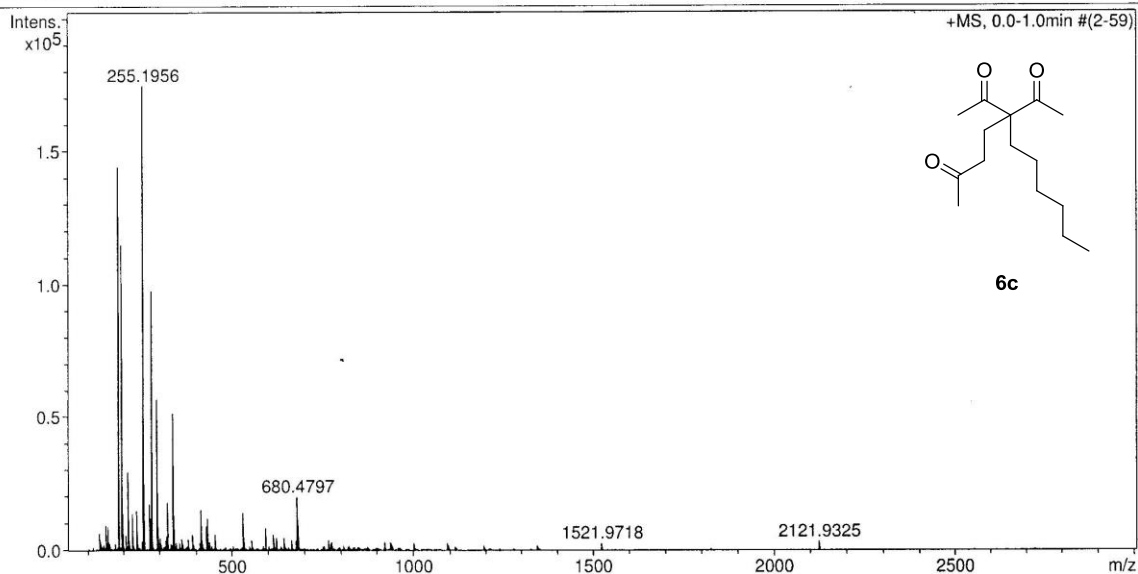
Analysis Name D:\Data\Chizhov\Nikishin\Terentiev\Wilbb-427\_&clblow.d  
Method tune\_low.m  
Sample Name /TERN BB-427  
Comment CH3CN 100 %, dil. 200, calibrant added

Acquisition Date 02.09.2013 16:02:57

Operator BDAL@DE  
Instrument / Ser# micrOTOF 10248

#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



## HRMS of 3-acetyl-3-[(4-chlorophenyl)methyl]heptane-2,6-dione (**6g**)

### Display Report

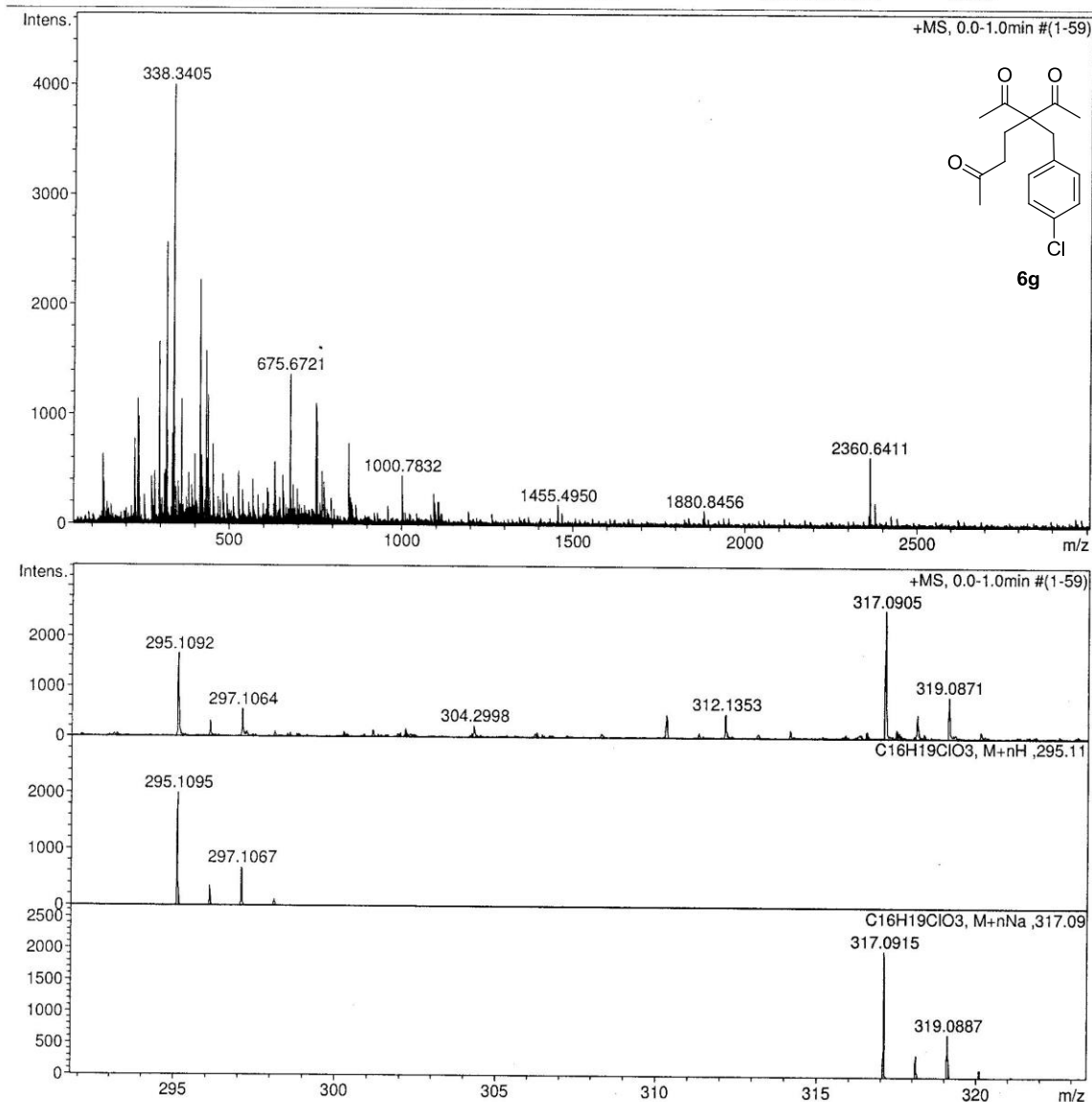
#### Analysis Info

Analysis Name D:\Data\Chizhov\Nikishin\Terentiev\Willbb-401\_low.d  
Method tune\_low.m  
Sample Name /TERN BB-401  
Comment CH<sub>3</sub>CN 100 %, dil. 200, no calibrant added

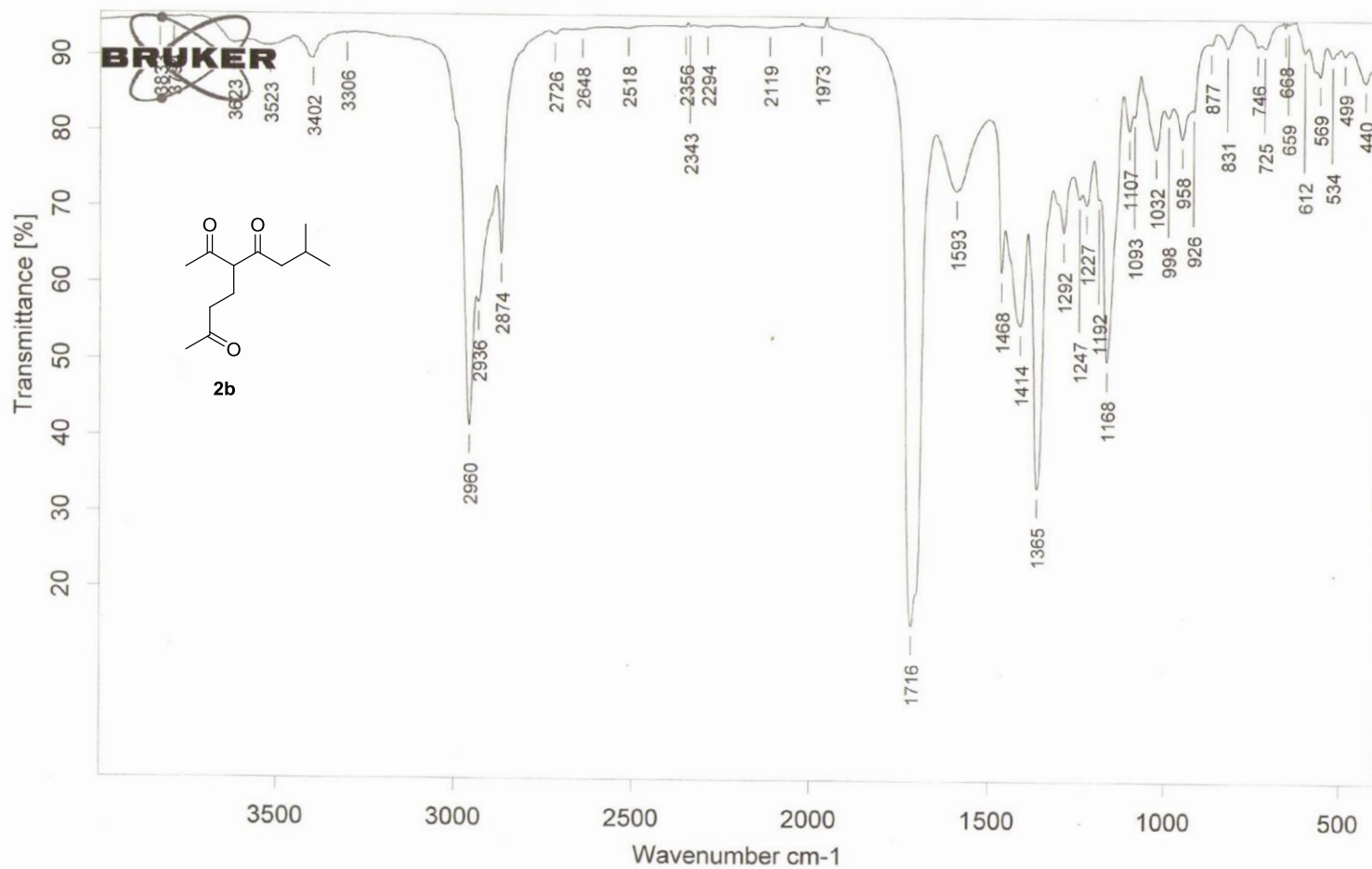
Acquisition Date 23.09.2013 16:14:20  
Operator BDAL@DE  
Instrument / Ser# micrOTOF 10248

#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



### IR of 5-acetyl-8-methylnonane-2,6-dione (**2b**)

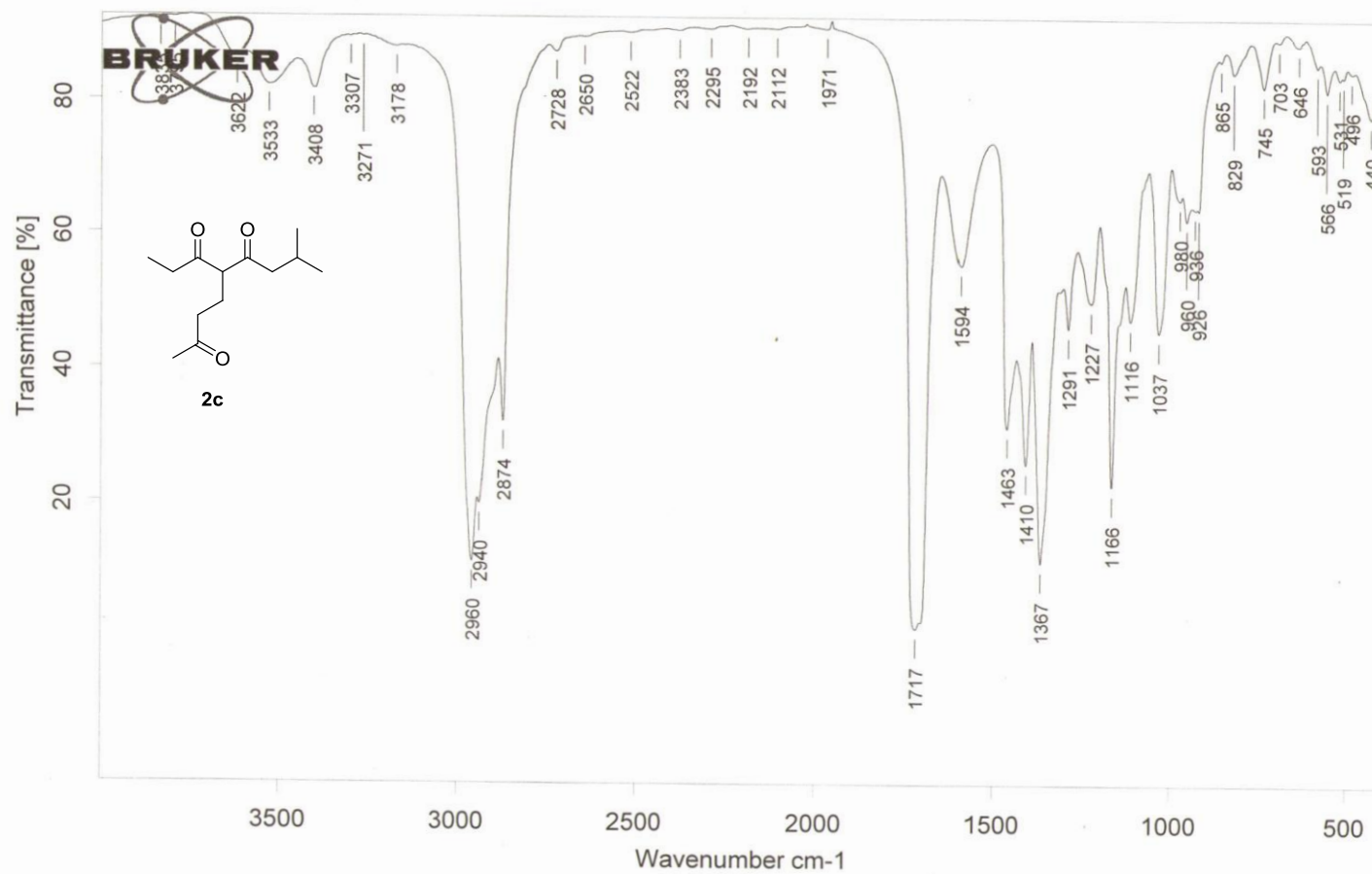


C:\OPUS\_7.0.122\EDL\VB-345.0

ВИЛЬ. ВВ-345, тонкий слой пл.КВг/

26.09.2013

### IR of 8-methyl-5-propionylnonane-2,6-dione (**2c**)

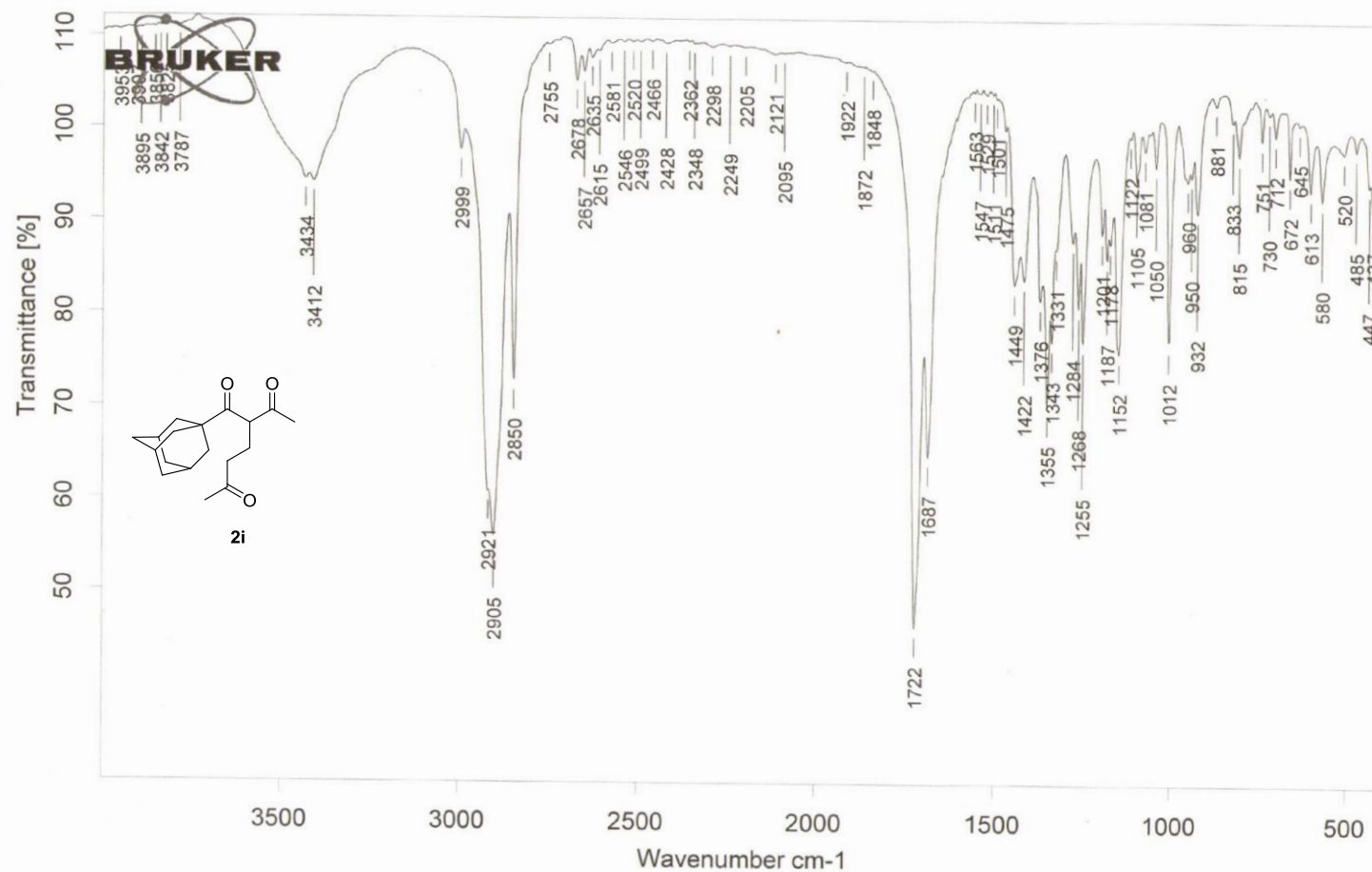


C:\OPUS\_7.0.122\EDL\VV-348.0

Виль. ВВ-348, тонкий слой пл.КВг/

26.09.2013

IR of 3-(adamant-1-ylcarbonyl)heptane-2,6-dione (**2i**)

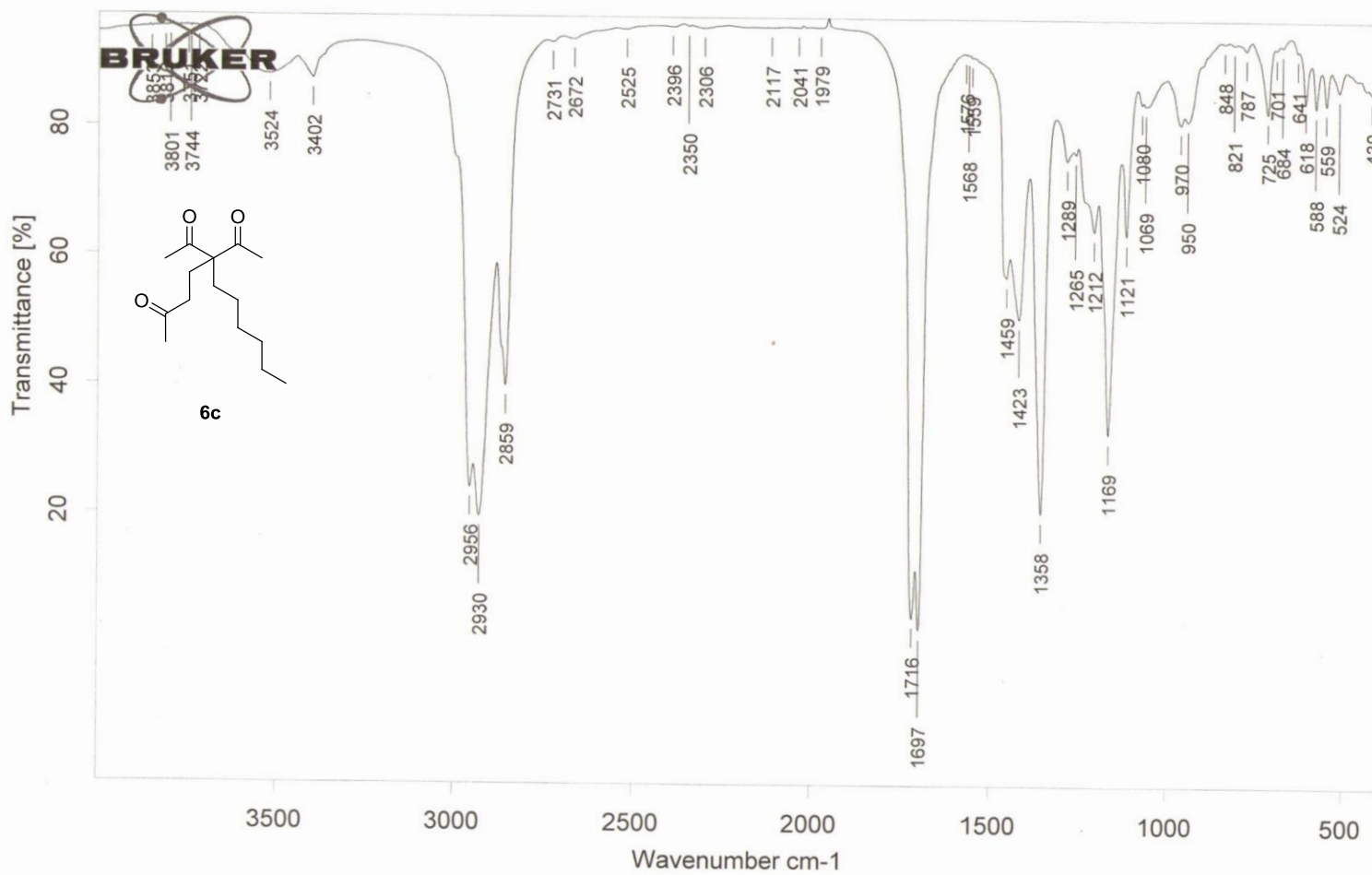


C:\OPUS\_7.0.122\EDL\B-291.0

ВИЛЬ. В-291, прессовка с KBr, 0.5/200.

26.09.2013

IR of 3-acetyl-3-hexylheptane-2,6-dione (**6c**)

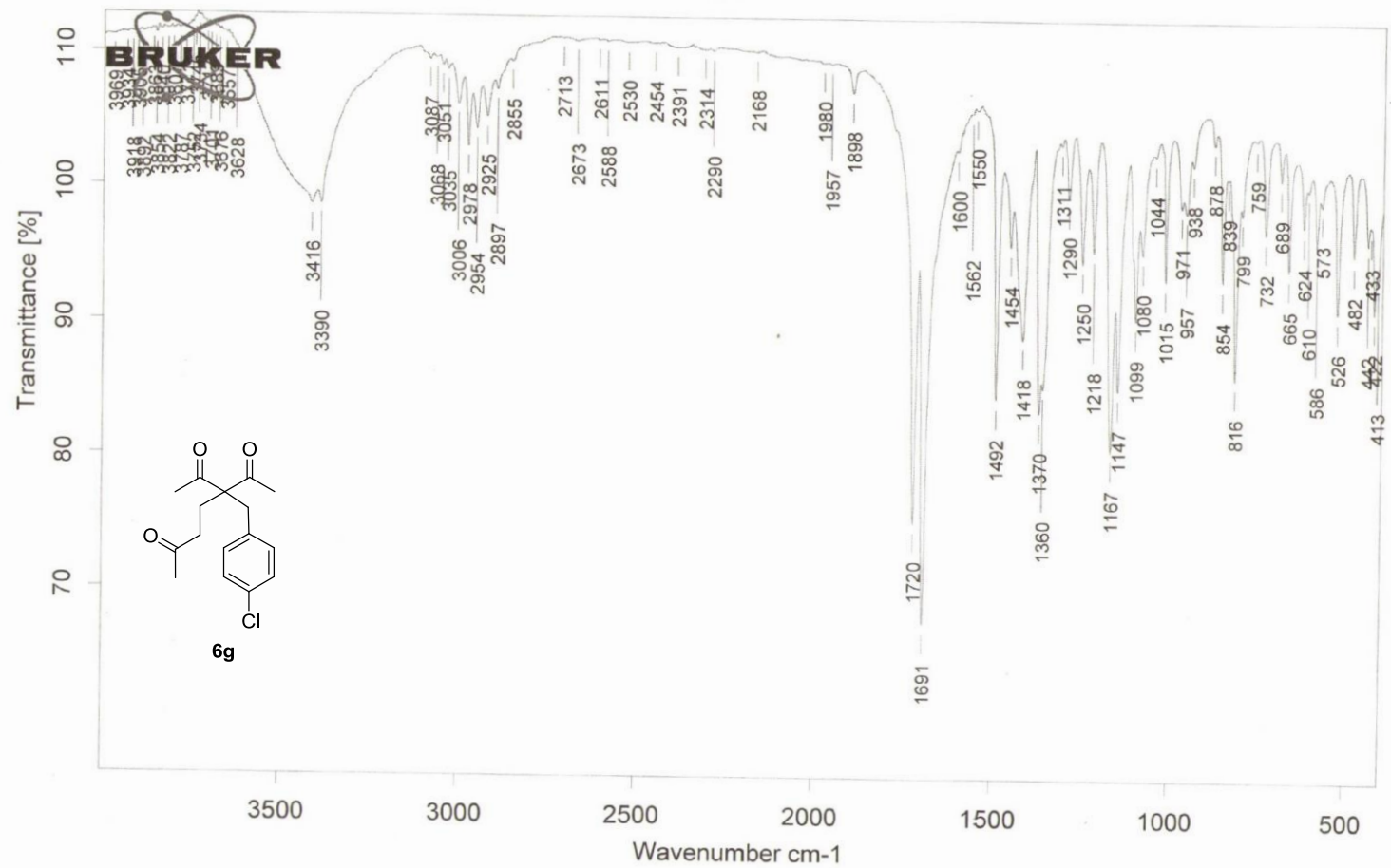


C:\OPUS\_7.0.122\EDL\BB-427.0

ВИЛЬ. ВВ-427, тонкий слой пл.КВг/

26.09.2013

IR of 3-acetyl-3-[(4-chlorophenyl)methyl]heptane-2,6-dione (**6g**)



C:\OPUS\_7.0.122\EDL\BB-401.0

ВИЛЬ. ВВ-401, прессовка с KBr, 0.5/200.

26.09.2013