Supplementary Material (ESI) for

Organic and Biomolecular Chemistry

Synthesis of 1-Hydroperoxy-1'-Alkoxyperoxides by the Iodine-Catalyzed Reactions of Geminal Bishydroperoxides with Acetals or Enol Ethers

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The molecular structure of **6d** has been confirmed by X-ray structure determination. Intensity data set was collected at room temperature using an Enraf-Nonius CAD4 diffractometer (Cu Kα radiation, λ = 1.54184 Å) equipped with a graphite monochromator. The crystal structure was solved by direct methods. Crystallographic programs used for structure solution and refinement, respectively, were *SHELXS97* and *SHELXL97* [1]. The structure was refined by full-matrix least-squares refinement on F^2. Hydrogen atoms were placed geometrically and refined using a riding model with U_{iso} constrained at 1.2 times U_{eq} of the carrier C or O atom. The crystal data, data collection and refinement parameters are given in Table.

Crystallographic data (excluding structure factors) for **6d** have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 689447. Copies of data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (44)1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).

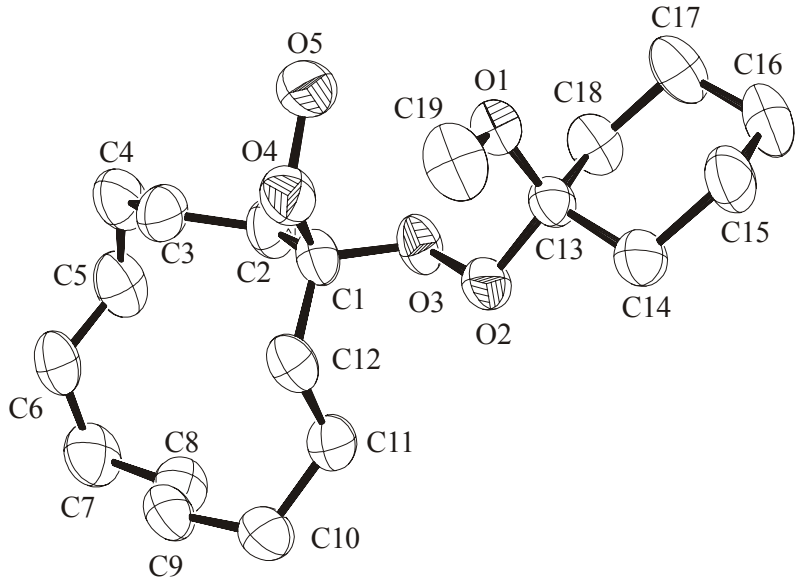

Fig. 1 The molecular structure of **6d**,

showing the atomic numbering and 50% probability displacement ellipsoids. H atoms omitted for clarity.

The molecular structure of **6d** drawn with ORTEP-III [2] is presented on Fig. 1. All bond lengths and angles are normal and comparable with those observed in two close compounds – 1,1-bis(hydroperoxy)cyclododecane [3, 4] and 1,1'-dihydroperoxy-1,1'-bis(cyclododecyl)peroxide [5, 6], respectively – found in the Cambridge Structural Database (CSD, Version 5.29 [7]). The hydroxy group in **6d** is involved in intramolecular O5-H5…O1 hydrogen bonding (D…A, H…A and D-H…A are 2.763(4) Å, 2.08 Å and 141^{o}, respectively). In the crystal, there are no intermolecular H…O contacts shorter than 2.75 Å, so crystal packing is typical of branched hydrocarbons, with hydrophobic space-filling contacts reflecting the simple close-packing of hydrophobic molecules [8, 9].

References.

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[5] P. Groth, *Acta Chem. Scand. A*, 1975, **29**, 783-786.

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[7] F.H. Allen, *Acta Cryst. B*, 2002, ***B58***, 380-388.

[8] F. Dubnikova, R. Kosloff, J. Almog, Y. Zeiri, R. Boese, H. Itzhaky, A. Alt, E. Keinan, *J. Am. Chem. Soc.,* 2005, **127**, 1146 -1159.

[9] A.O. Terent'ev, M.M. Platonov, A.I. Tursina, V.V. Chernyshev, G.I. Nikishin, *J. Org. Chem.,* 2008, **73**, 3169-3174.

Table. Crystal data for **6d**.

1-Hydroperoxy-1-(1-methoxycyclohexylperoxy)cyclododecane, 6d	
empirical formula	$C_{19}H_{36}O_5$
M_r	344.48
crystal size, mm^3	0.22 x 0.21 x 0.07
crystal form, colour	plate, colourless
crystal system	triclinic
space group	P-1
unit cell dimensions	
a, Å	8.3859(13)
b, Å	10.9820(14)
c, Å	11.3351(16)
α, ^{o}	109.105(11)
β, ^{o}	95.714(12)
γ, ^{o}	93.578(12)
volume, $Å^3$	976.5(3)
Z	2
μ, mm^{-1}	0.666
no. reflns collected/independent	3904/3703 [$R(int)$ = 0.0372]
no. params	218
GOF	0.936
final R indices [$I>2\sigma(I)$]	R = 0.0518, wR = 0.1215

1-[(1-ethoxycyclopentyl)peroxy]cyclohexyl hydroperoxide ***(3c)***

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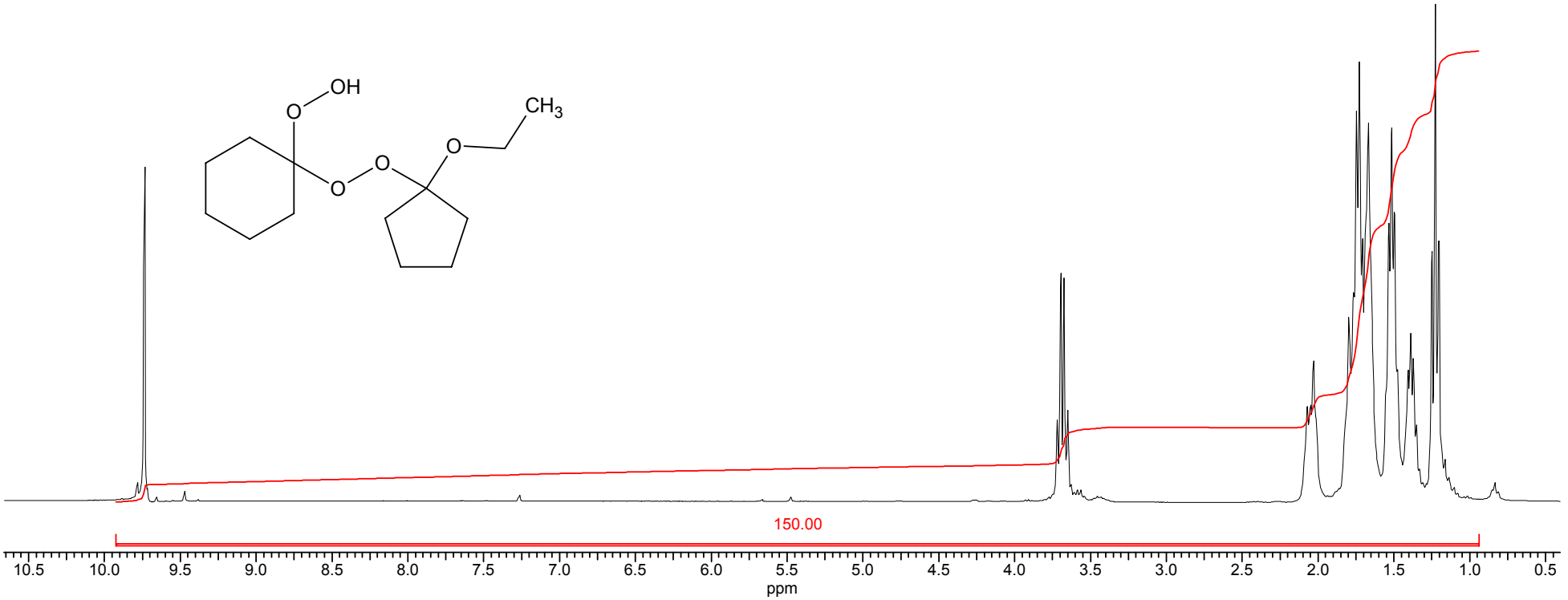

No.	(ppm)	Value
1	.94 .. 9.9	150.000

1-[(1-ethoxycyclopentyl)peroxy]cyclohexyl hydroperoxide ***(3c)***

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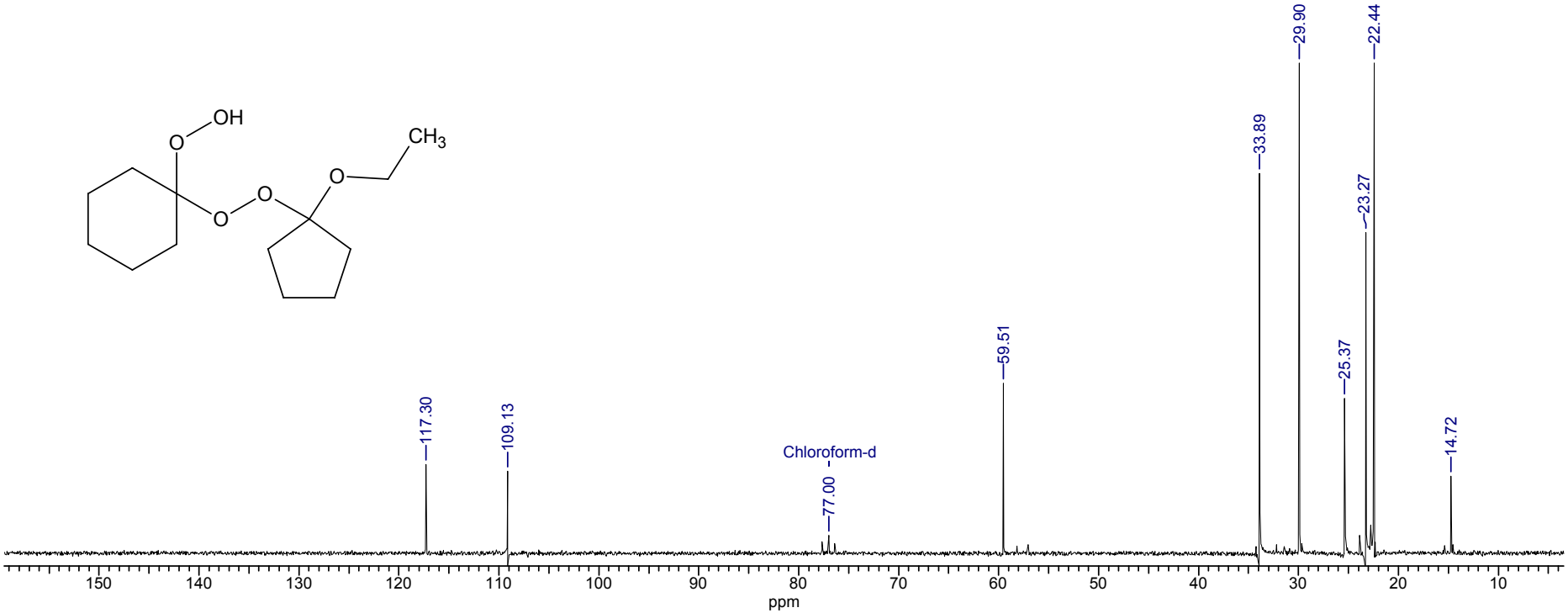

No.	(ppm)	(Hz)	Height
1	14.72	740.9	0.1575
2	22.44	1129.5	0.9998
3	23.27	1171.2	0.6538
4	25.37	1276.9	0.3160
5	29.90	1504.7	1.0000
6	33.89	1705.7	0.7752
7	59.51	2995.0	0.3468
8	77.00	3874.9	0.0363
9	109.13	5491.8	0.1667
10	117.30	5902.7	0.1813

No.	Annotation	(ppm)
1	Chloroform-d	77.00

1-[(1-methoxycyclohexyl)peroxy]cyclohexyl hydroperoxide ***(3d)***

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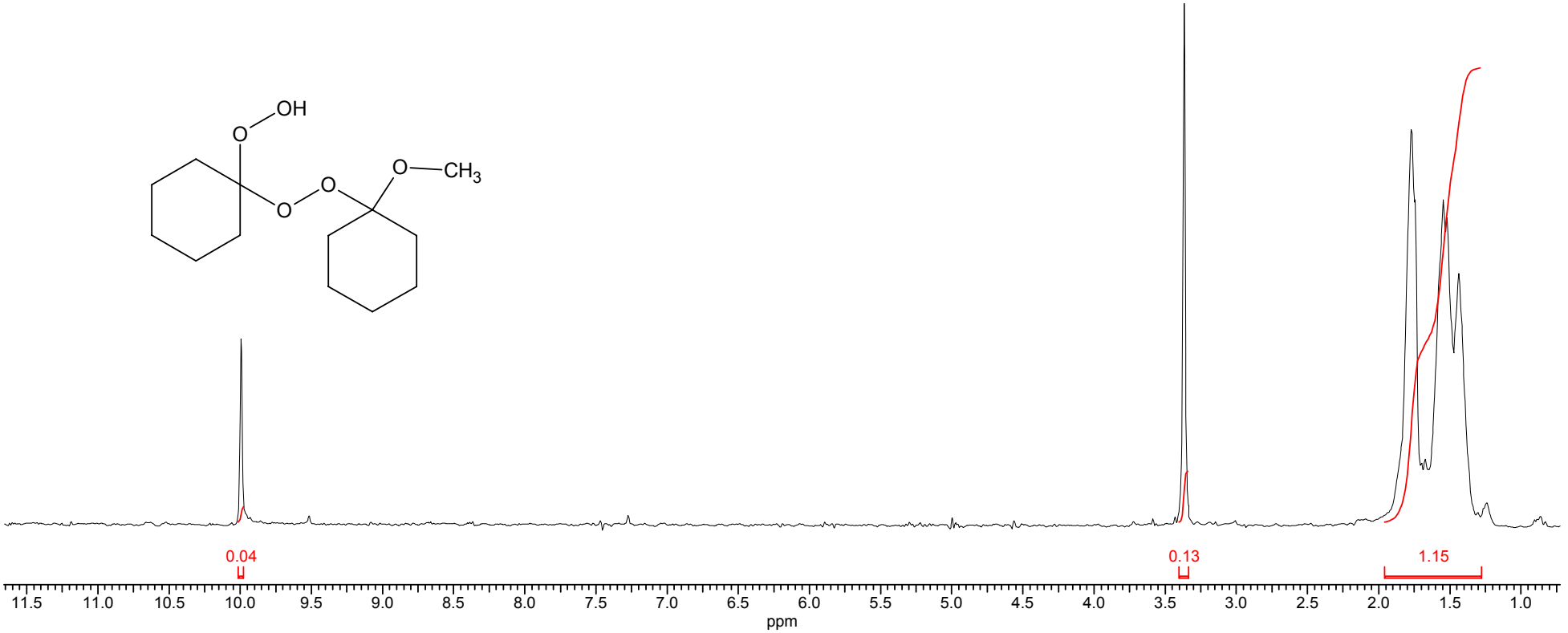
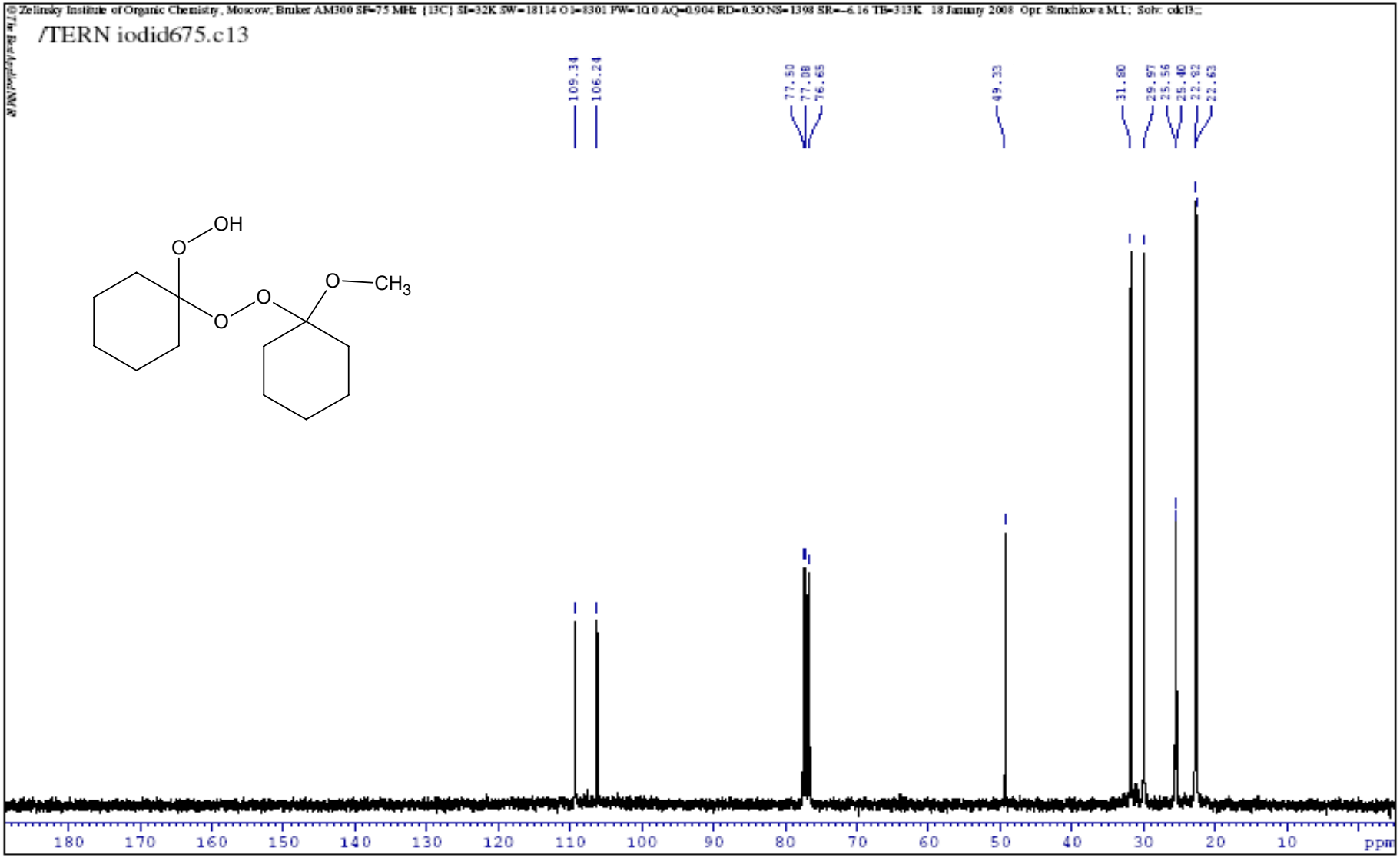
Solvent	DMSO-D6	***Sweep Width (Hz)***	4000.00	***Temperature (degree C)***	24.000		



No.	(ppm)	Value
1	.28 .. 1.9	1.150
2	.34 .. 3.4	0.131
3	98 .. 10.0	0.040

1-[(1-methoxycyclohexyl)peroxy]cyclohexyl hydroperoxide ***(3d)***



1-[(1-methoxycycloheptyl)peroxy]cyclohexyl hydroperoxide ***(3e)***

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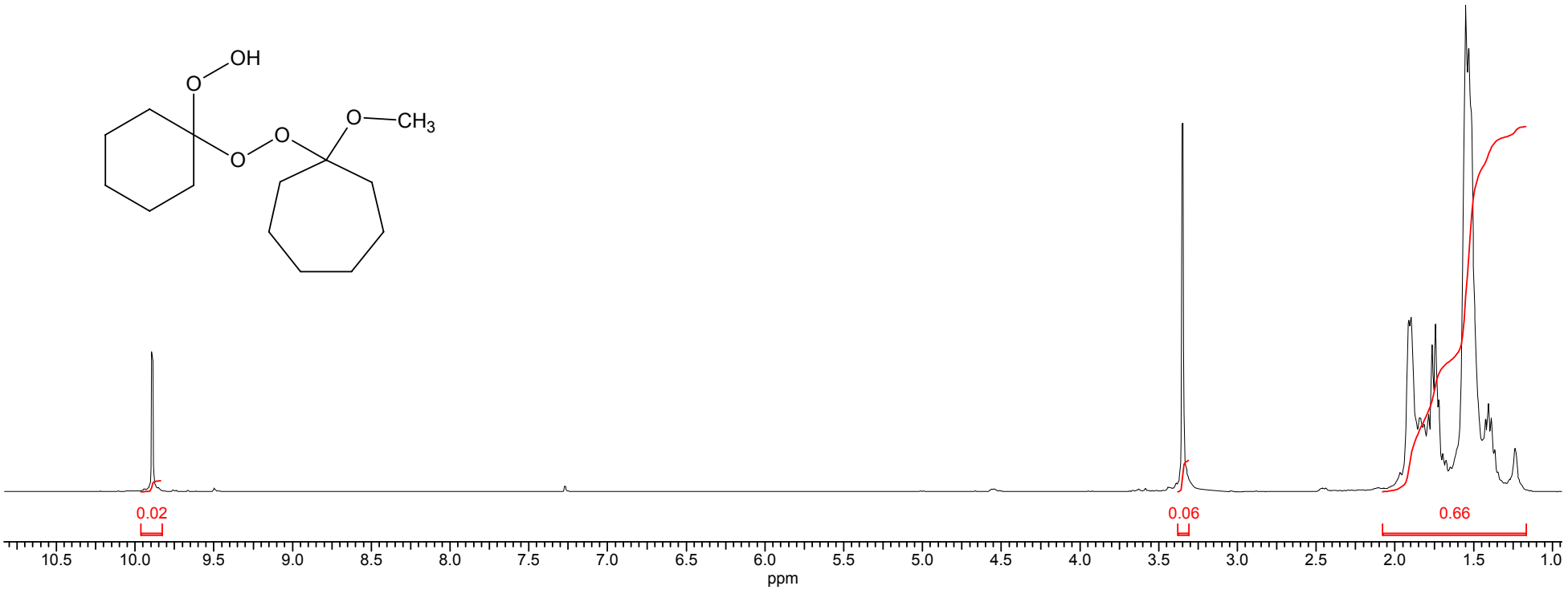
Temperature (degree C)	35.300						



No.	(ppm)	Value
1	[9.83 .. 9.96]	0.020
2	[3.31 .. 3.38]	0.057
3	[1.17 .. 2.08]	0.656

1-[(1-methoxycycloheptyl)peroxy]cyclohexyl hydroperoxide ***(3e)***

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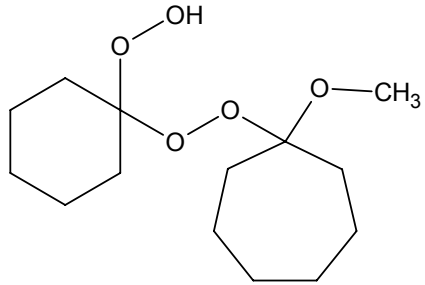
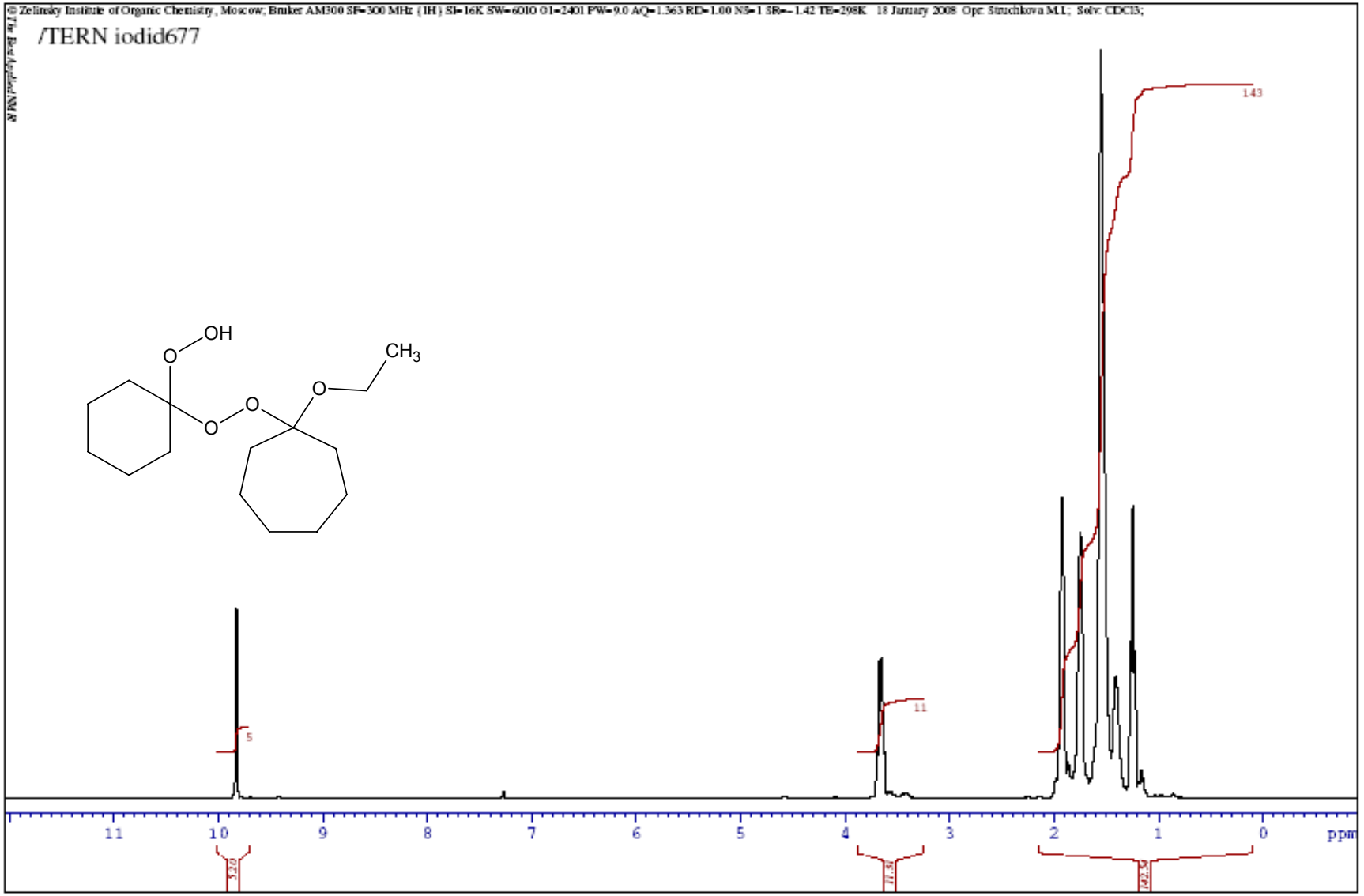


No.	(ppm)	(Hz)	Height
1	22.24	1119.1	0.3224
2	22.36	1125.0	0.2475
3	22.47	1131.0	1.0000
4	25.40	1278.4	0.4897
5	29.57	1488.3	0.3126
6	29.84	1501.7	0.8985
7	29.90	1504.7	0.2251

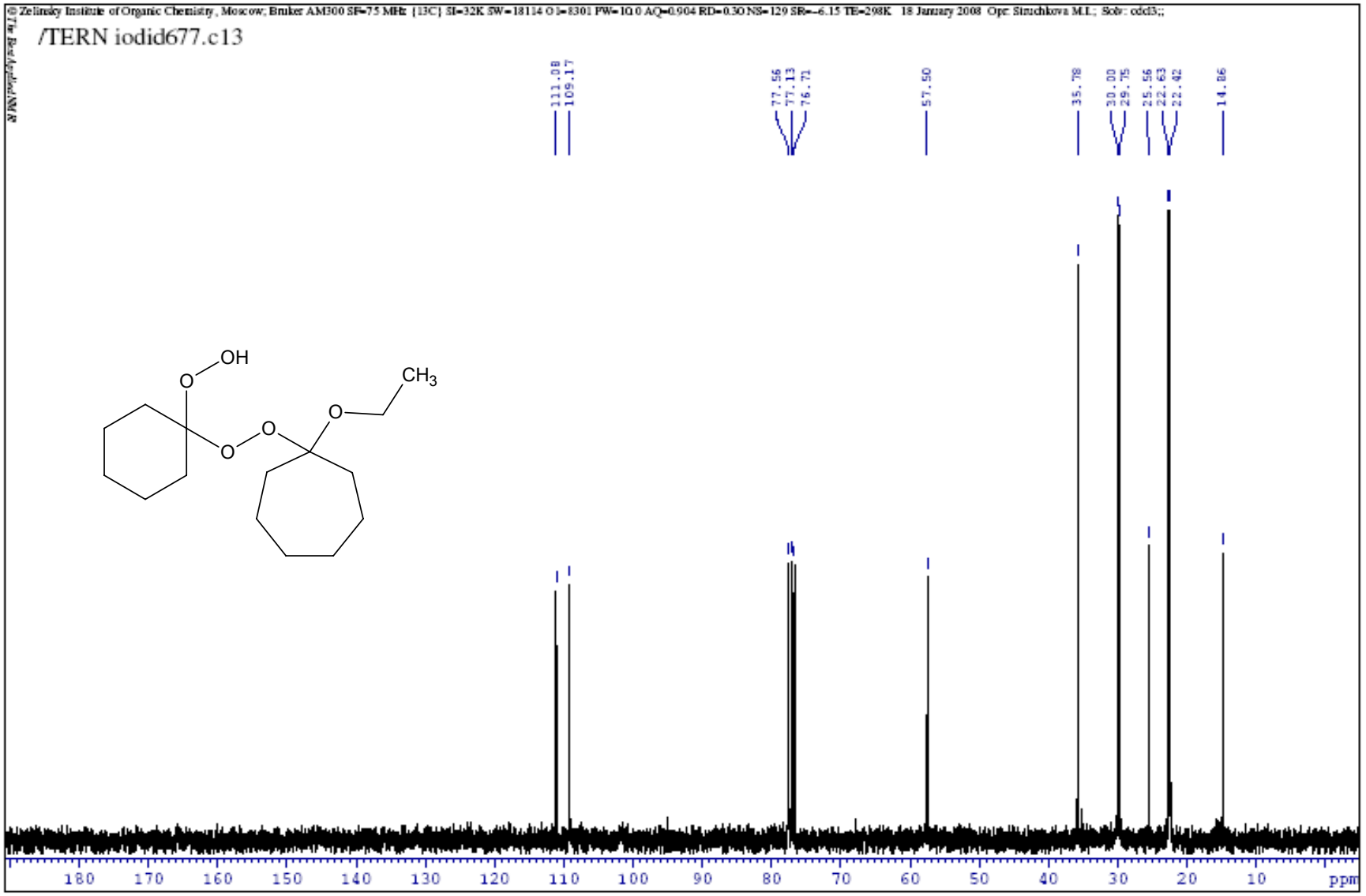
No.	(ppm)	(Hz)	Height
8	34.60	1741.4	0.2551
9	35.08	1765.2	0.4277
10	49.57	2494.8	0.1882
11	77.00	3874.9	0.0670
12	109.28	5499.2	0.1623
13	111.02	5587.1	0.1653

No.	Annotation	(ppm)
1	Chloroform-d	77.00

1-[(1-ethoxycycloheptyl)peroxy]cyclohexyl hydroperoxide ***(3f)***



1-[(1-ethoxycycloheptyl)peroxy]cyclohexyl hydroperoxide ***(3f)***



1-[(1-methoxy-1-methylethyl)peroxy]-4-methylcyclohexyl hydroperoxide ***(4a)***

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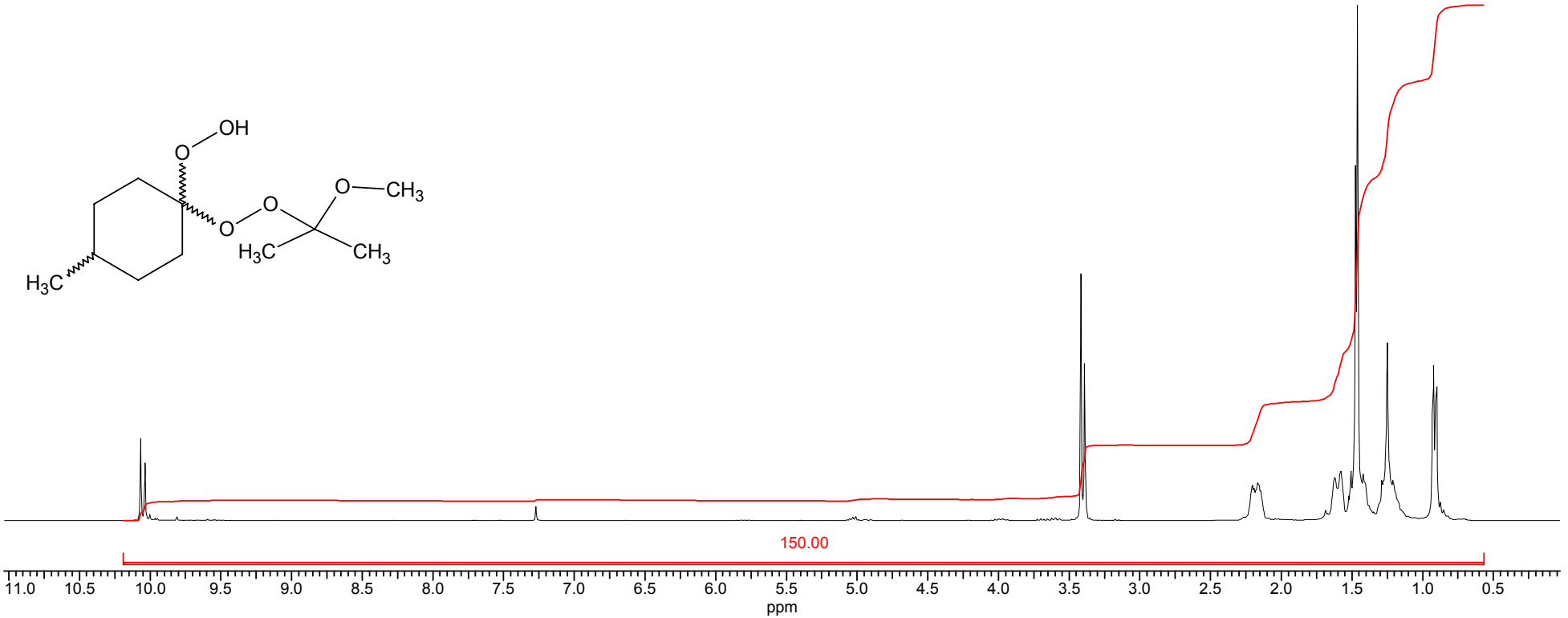
Temperature (degree C)	22.500						



No.	(ppm)	Value
1	57 .. 10.1	150.000

1-[(1-methoxy-1-methylethyl)peroxy]-4-methylcyclohexyl hydroperoxide ***(4a)***

Acquisition Time (sec)	0.4501	***Comment***	Avance-300, C-13, CDCl3			***Date***	20 Feb 2008 12:54:24
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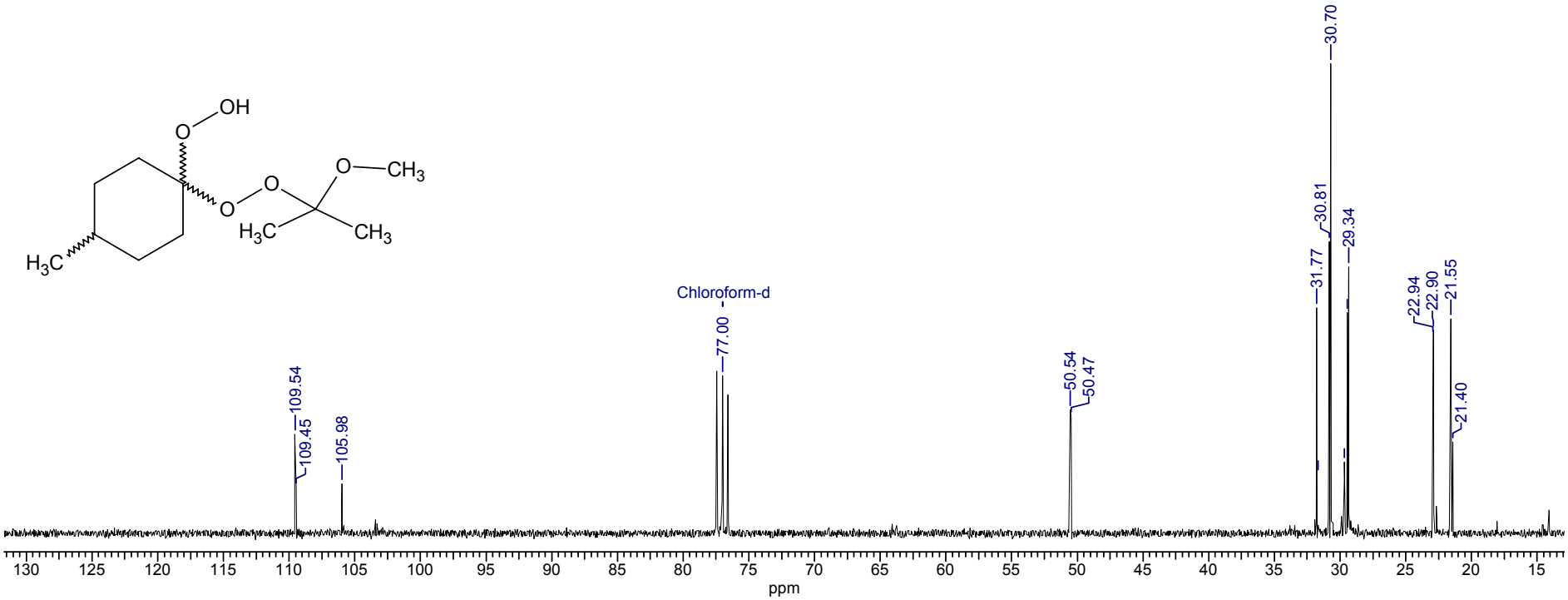
Temperature (degree C)	22.600						



No.	(ppm)	(Hz)	Height
1	21.40	1615.3	0.1948
2	21.55	1626.3	0.4567
3	22.90	1728.0	0.4329
4	22.94	1731.4	0.4212
5	29.34	2214.6	0.5671
6	29.44	2222.3	0.4701
7	29.66	2238.9	0.1526
8	30.70	2317.4	1.0000
9	30.81	2325.2	0.6214

No.	(ppm)	(Hz)	Height
10	31.67	2390.4	0.1264
11	31.77	2398.2	0.4805
12	50.47	3809.1	0.2500
13	50.54	3814.7	0.2635
14	77.00	5811.7	0.3359
15	105.98	7998.9	0.1054
16	109.45	8261.0	0.0981
17	109.54	8267.6	0.2118

No.	Annotation	(ppm)
1	Chloroform-d	77.00

1-[(1-methoxy-1-methyloctyl)peroxy]-4-methylcyclohexyl hydroperoxide ***(4b)***

Acquisition Time (sec)	1.0240	***Comment***	/TERN IODID686 Opr:Struchkova M.I.;Solv:CDCl3;			***Date***	23/01/2008 17:53:42
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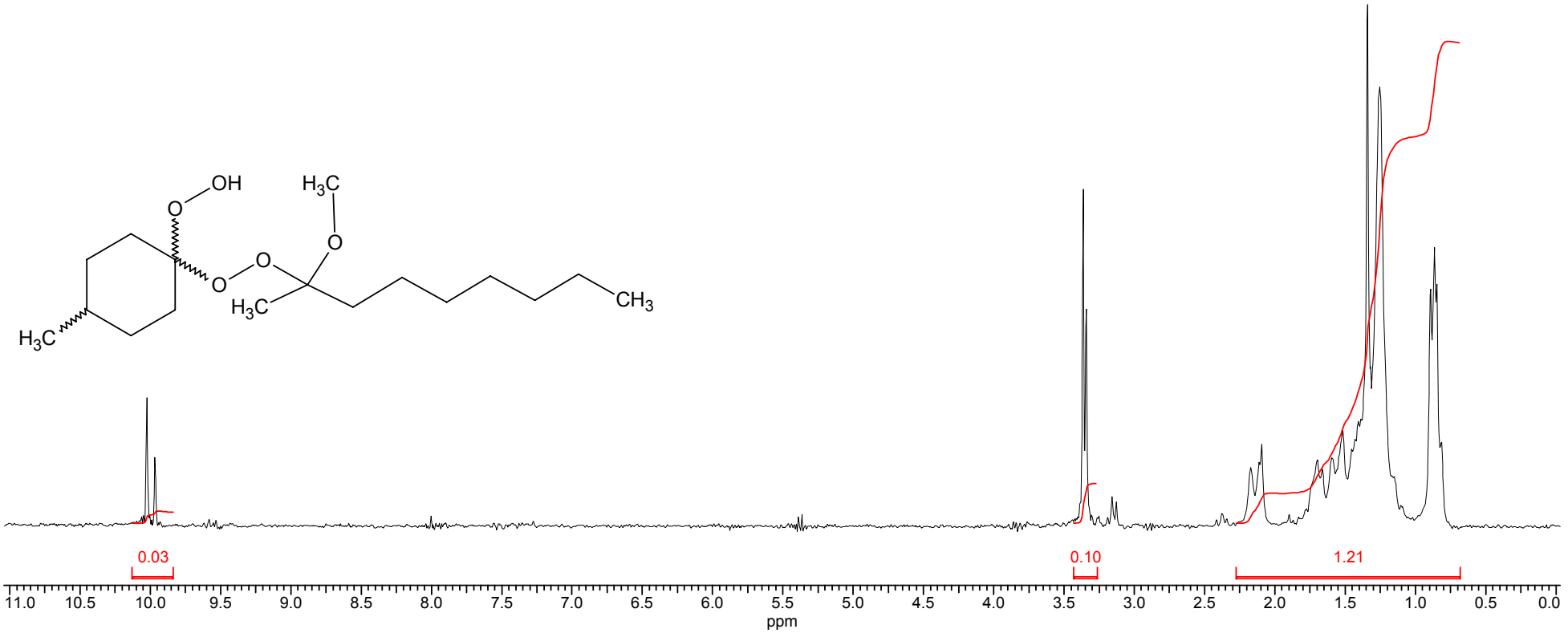
Solvent	DMSO-D6	***Sweep Width (Hz)***	4000.00	***Temperature (degree C)***	24.000		



No.	(ppm)	Value
1	.68 .. 2.2	1.215
2	.26 .. 3.4	0.102
3	84 .. 10.1	0.028

1-[(1-methoxy-1-methyloctyl)peroxy]-4-methylcyclohexyl hydroperoxide ***(4b)***

Acquisition Time (sec)	0.3359	***Comment***	/TERN IODID686.C13□Opr:Struchkova M.I.;Solv:CDCl3;	***Date***	23/01/2008 18:37:46
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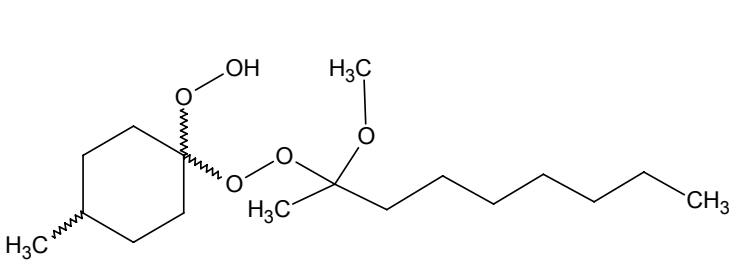

No.	(ppm)	(Hz)	Height
1	13.95	702.2	0.3210
2	19.55	983.6	0.1912
3	19.63	988.0	0.6181
4	21.38	1075.9	0.3528
5	21.47	1080.3	0.6648
6	22.53	1133.9	0.9725
7	24.16	1215.8	0.5398
8	29.04	1461.5	0.7513
9	29.10	1464.5	0.5277
10	29.16	1467.4	0.4646
11	29.40	1479.4	0.4884
12	29.63	1491.3	1.0000

No.	(ppm)	(Hz)	Height
13	30.64	1541.9	0.8083
14	30.85	1552.3	0.2789
15	31.65	1592.5	0.7427
16	35.64	1793.5	0.5206
17	35.73	1798.0	0.2185
18	49.99	2515.6	0.1568
19	50.08	2520.1	0.7334
20	77.00	3874.9	0.1531
21	107.92	5430.8	0.3214
22	109.19	5494.8	0.1908
23	109.31	5500.7	0.3458

No.	Annotation	(ppm)
1	Chloroform-d	77.00

1-[(1-methoxy-1-methyloctyl)peroxy]-4-methylcyclohexyl hydroperoxide ***(4b)***

Acquisition Time (sec)	0.3523	***Comment***	/TERN IODID686.J□Opr:Struchkova M.I.;Solv:CDCl3;			***Date***	23/01/2008 18:57:47
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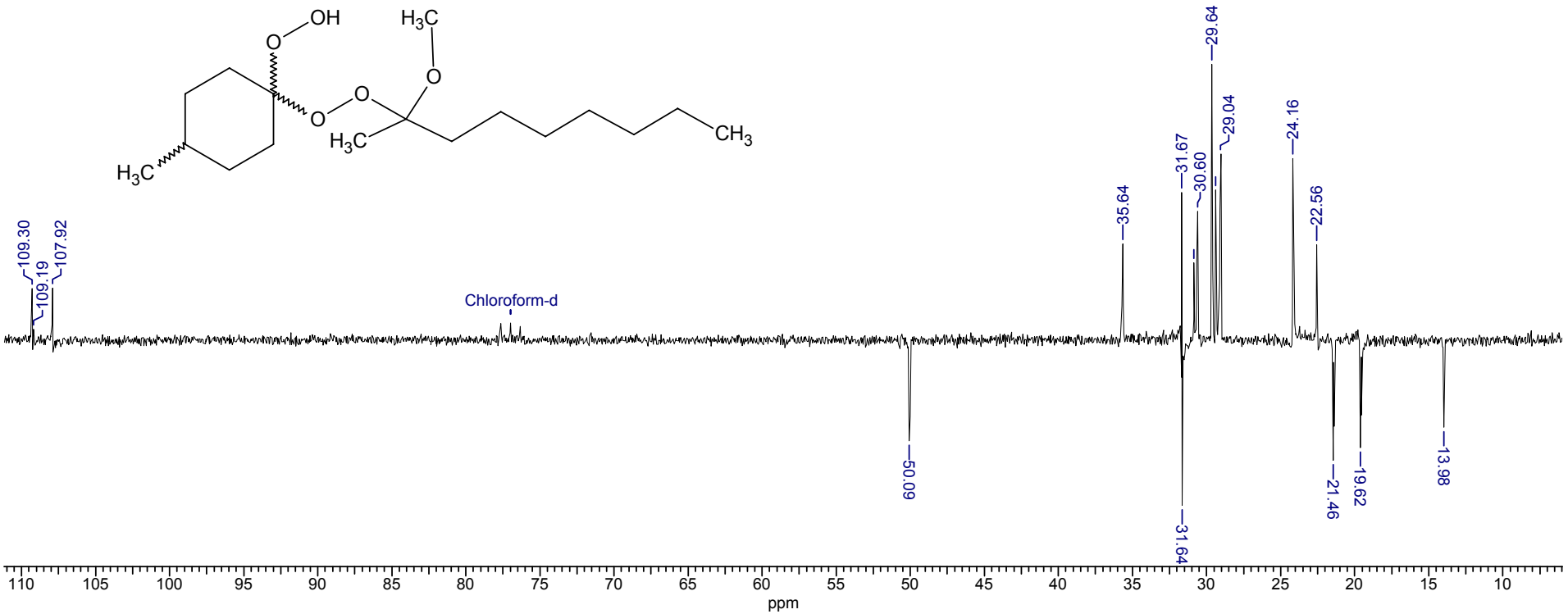

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3	21.46	1079.7	-0.4366
4	22.56	1135.1	0.3441
5	24.16	1216.0	0.6589
6	29.04	1461.6	0.6748
7	29.38	1478.6	0.5432
8	29.64	1491.4	1.0000
9	30.60	1539.7	0.4666

No.	(ppm)	(Hz)	Height
10	30.85	1552.4	0.2793
11	31.64	1592.2	-0.6009
12	31.67	1593.6	0.5351
13	35.64	1793.8	0.3484
14	50.09	2520.6	-0.3669
15	107.92	5430.8	0.1880
16	109.19	5494.7	0.0384
17	109.30	5500.3	0.1869

No.	Annotation	(ppm)
1	Chloroform-d	77.00

1-[(1-ethoxycyclopentyl)peroxy]-4-methylcyclohexyl hydroperoxide ***(4c)***

Acquisition Time (sec)	0.6759	***Comment***	levc;091	***Date***	08 Feb 2008 14:28:16		
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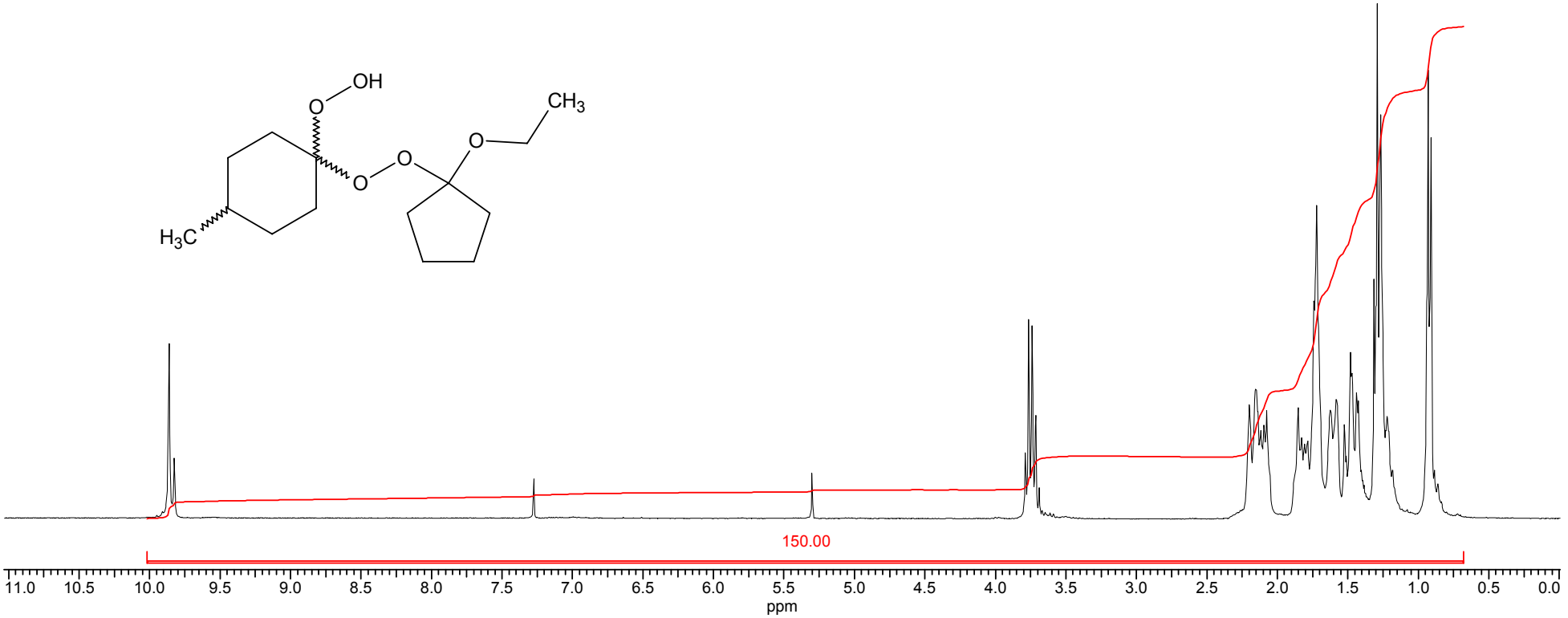
Temperature (degree C)	30.100						



No.	(ppm)	Value
1	68 .. 10.0	150.000

1-[(1-ethoxycyclopentyl)peroxy]-4-methylcyclohexyl hydroperoxide ***(4c)***

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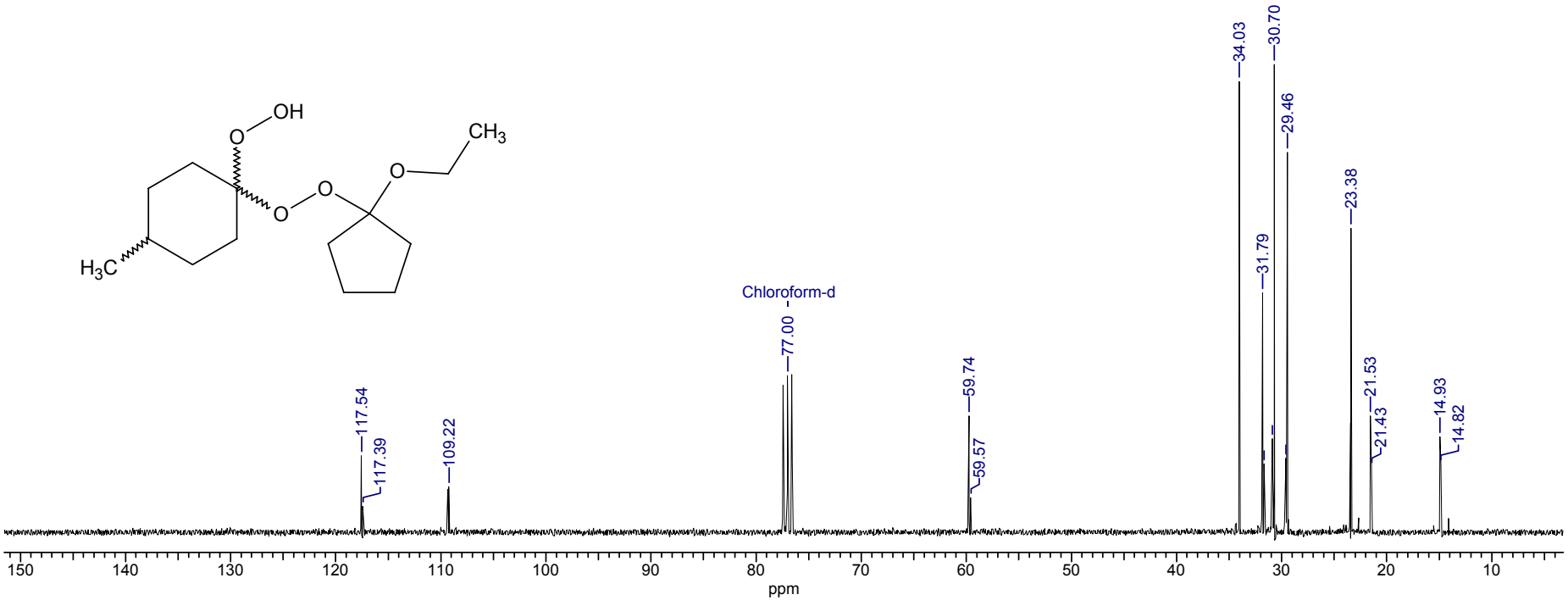
Points Count	16384	***Pulse Sequence***	zgpg30base	***Solvent***	CHLOROFORM-D	***Sweep Width (Hz)***	18115.94
Temperature (degree C)	20.100						



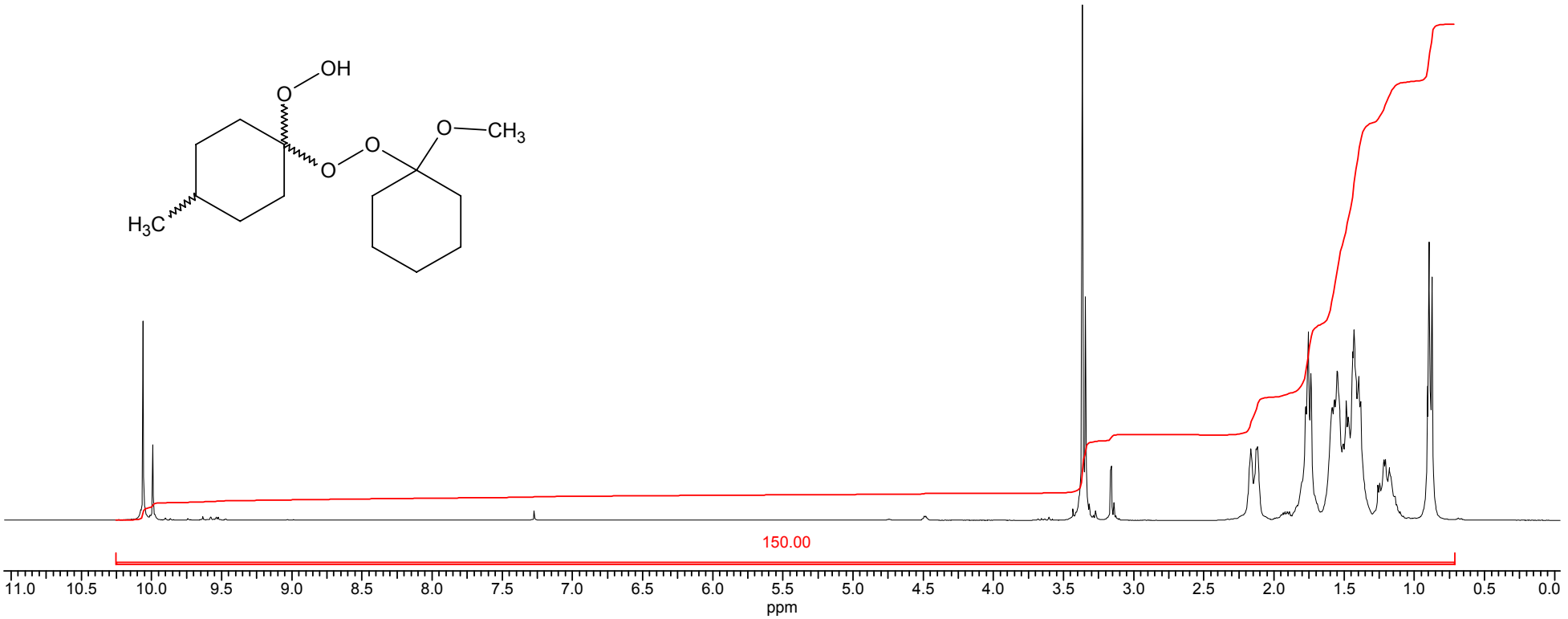
No.	(ppm)	(Hz)	Height
1	14.82	1118.8	0.1461
2	14.93	1126.5	0.2037
3	21.43	1617.5	0.1400
4	21.53	1625.2	0.2492
5	23.38	1764.5	0.6503
6	23.45	1770.1	0.2339
7	29.46	2223.4	0.8124
8	29.58	2232.3	0.1586
9	30.70	2317.4	1.0000
10	30.87	2329.6	0.1998

No.	(ppm)	(Hz)	Height
11	31.69	2391.5	0.1460
12	31.79	2399.2	0.5120
13	34.03	2568.4	0.9636
14	59.57	4495.8	0.0746
15	59.74	4509.1	0.2491
16	77.00	5811.7	0.3348
17	109.22	8243.3	0.0977
18	109.31	8249.9	0.0920
19	117.39	8860.3	0.0558
20	117.54	8871.4	0.1637

No.	Annotation	(ppm)
1	Chloroform-d	77.00

1-[(1-methoxycyclohexyl)peroxy]-4-methylcyclohexyl hydroperoxide ***(4d)***

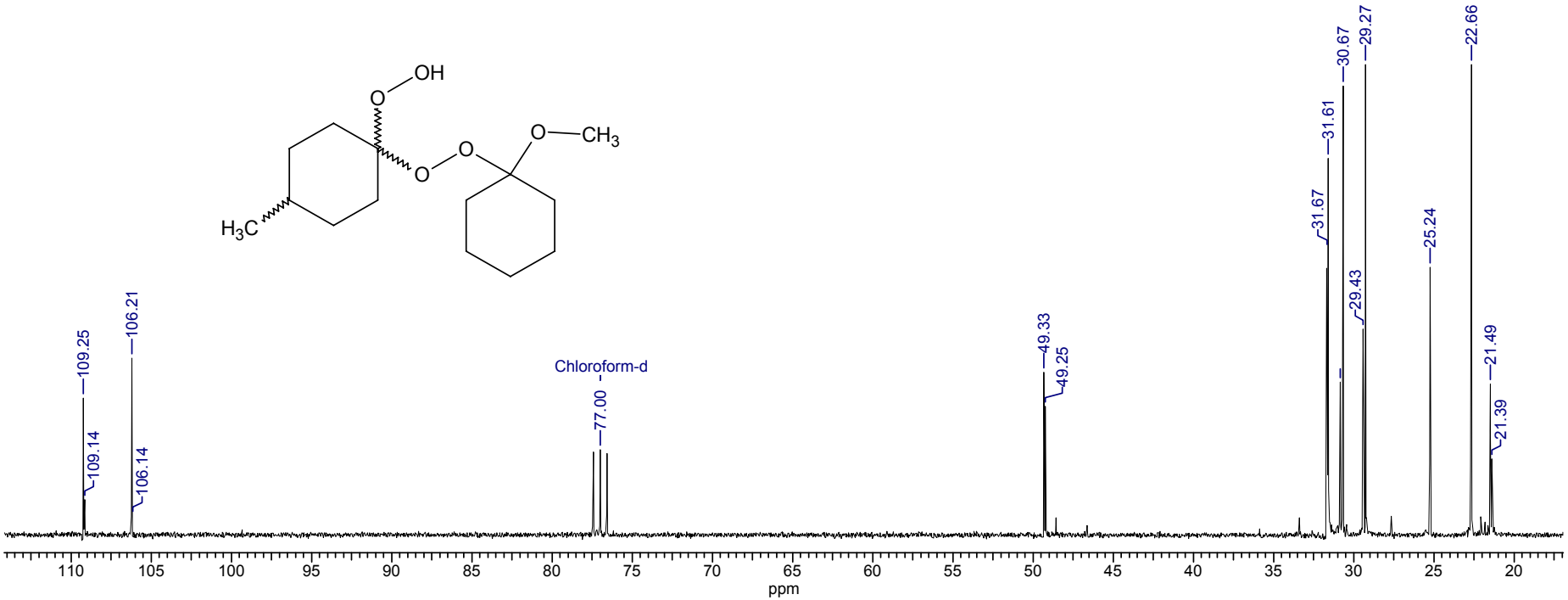
Acquisition Time (sec)	0.6759	***Comment***	Avance-300, CDCl3	***Date***	10 Jan 2008 09:08:16		
File Name	C:\Documents and Settings\Пользователь\Мои документы\Документы Платонов\Спектры фиды\tern\iodid650.001.{1H}\iodid650.001.{1H}_001000fid						
Frequency (MHz)	300.13	***Nucleus***	1H	***Number of Transients***	1	***Original Points Count***	8124
Points Count	8192	***Pulse Sequence***	zg	***Solvent***	CHLOROFORM-D	***Sweep Width (Hz)***	6009.62
Temperature (degree C)	22.900						



No.	(ppm)	Value
1	71 .. 10.2	150.000

1-[(1-methoxycyclohexyl)peroxy]-4-methylcyclohexyl hydroperoxide ***(4d)***

Acquisition Time (sec)	0.4501	***Comment***	Avance-300, C-13, CDCl3			***Date***	10 Jan 2008 09:10:24
File Name	C:\Documents and Settings\Пользователь\Мои документы\Документы Платонов\Спектры фиды\tern\iodid650.013.{13C}\iodid650.013.{13C}_013000fid						
Frequency (MHz)	75.48	***Nucleus***	13C	***Number of Transients***	661	***Original Points Count***	16308
Points Count	16384	***Pulse Sequence***	zgpg30base	***Solvent***	CHLOROFORM-D	***Sweep Width (Hz)***	18115.94
Temperature (degree C)	23.000						



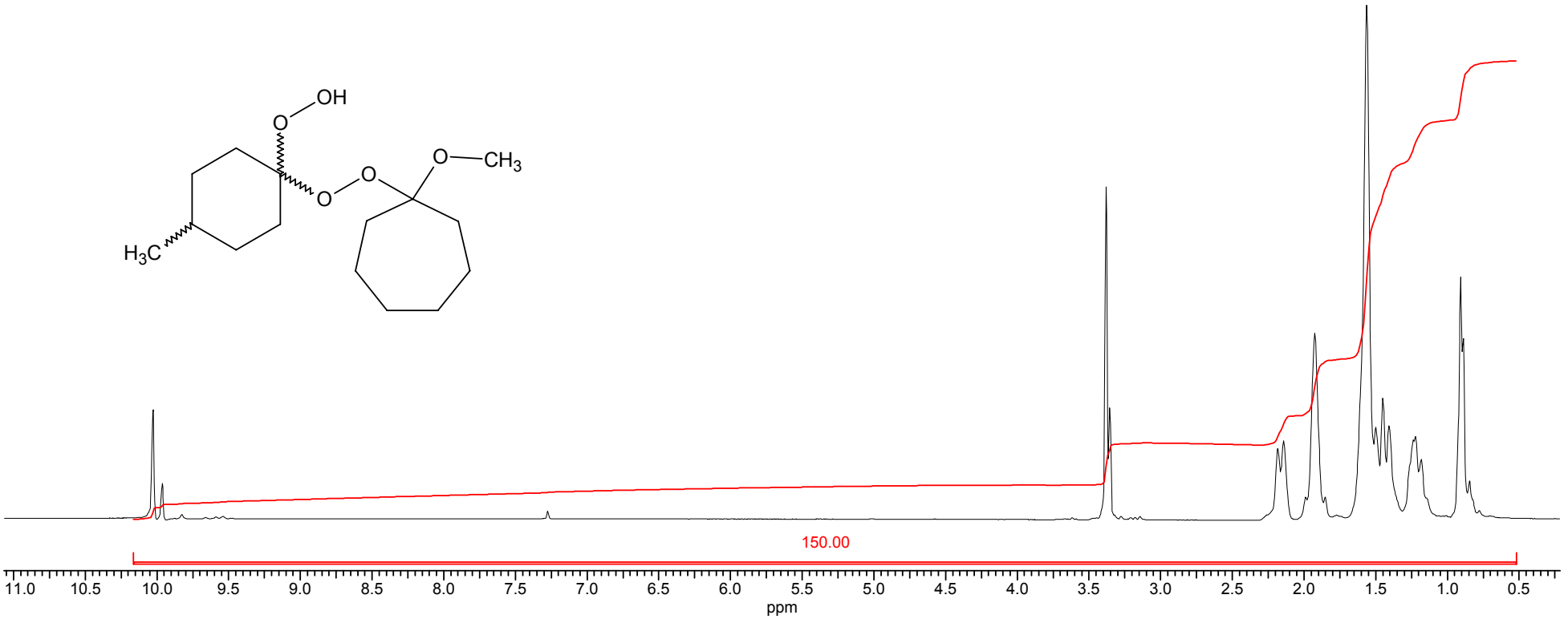
No.	(ppm)	(Hz)	Height
1	21.39	1614.1	0.1623
2	21.49	1621.9	0.3211
3	22.66	1710.3	0.9999
4	22.70	1713.7	0.3034
5	25.24	1905.0	0.5692
6	25.28	1908.3	0.1525
7	29.27	2209.1	1.0000
8	29.43	2221.2	0.4378
9	30.67	2315.2	0.9551
10	30.85	2328.5	0.3261

No.	(ppm)	(Hz)	Height
11	31.61	2386.0	0.8013
12	31.67	2390.4	0.6082
13	31.70	2392.6	0.5674
14	49.25	3717.3	0.2740
15	49.33	3722.9	0.3463
16	77.00	5811.7	0.1822
17	106.14	8011.1	0.0420
18	106.21	8016.6	0.3761
19	109.14	8237.7	0.0761
20	109.25	8245.5	0.2912

No.	Annotation	(ppm)
1	Chloroform-d	77.00

1-[(1-methoxycycloheptyl)peroxy]-4-methylcyclohexyl hydroperoxide ***(4e)***

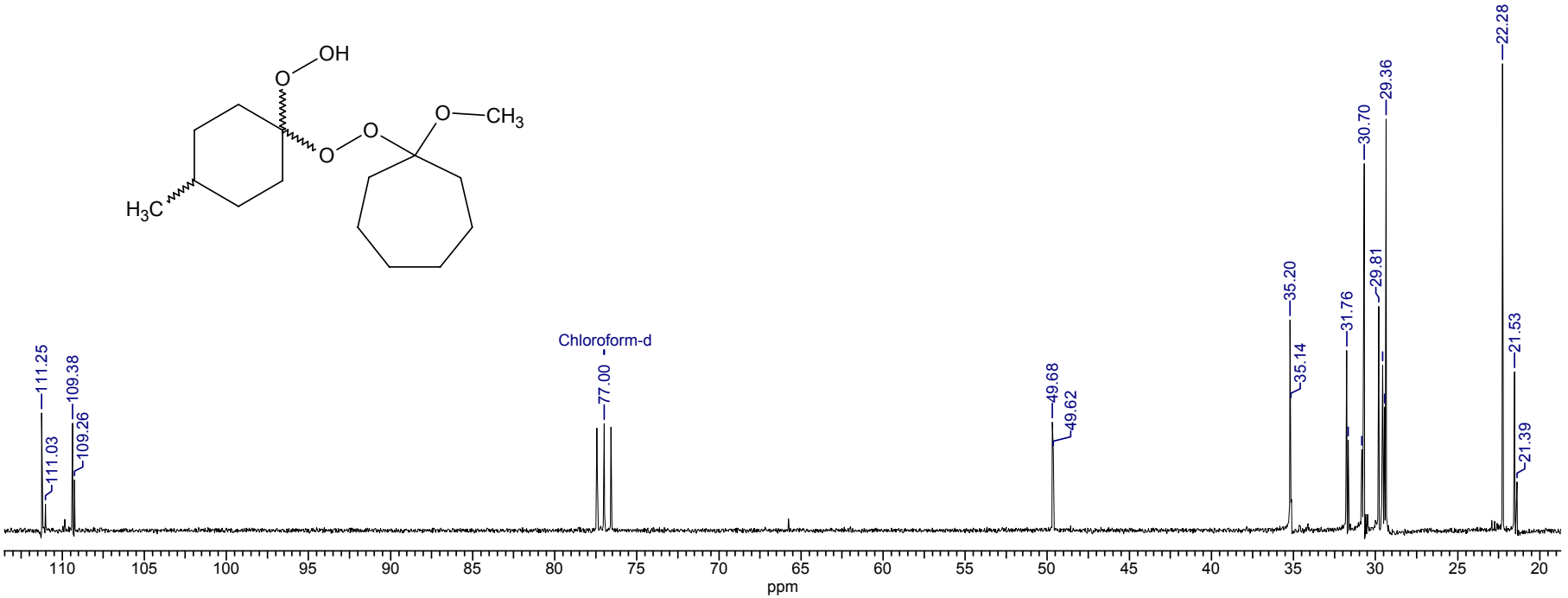
Acquisition Time (sec)	0.6759	***Comment***	Avance-300, CDCl3	***Date***	14 Jan 2008 14:13:20		
File Name	C:\Documents and Settings\Пользователь\Мои документы\Документы Платонов\Спектры фиды\tern\iodid658.001.{1H}\iodid658.001.{1H}_001000fid						
Frequency (MHz)	300.13	***Nucleus***	1H	***Number of Transients***	1	***Original Points Count***	8124
Points Count	8192	***Pulse Sequence***	zg	***Solvent***	CHLOROFORM-D	***Sweep Width (Hz)***	6009.62
Temperature (degree C)	24.400						



No.	(ppm)	Value
1	52 .. 10.1	150.000

1-[(1-methoxycycloheptyl)peroxy]-4-methylcyclohexyl hydroperoxide ***(4e)***

Acquisition Time (sec)	0.4501	***Comment***	Avance-300, C-13, CDCl3			***Date***	15 Jan 2008 11:01:20
File Name	C:\Documents and Settings\Пользователь\Мои документы\Документы Платонов\Спектры фиды\tern\iodid658.013.{13C}\iodid658.013.{13C}_013000fid						
Frequency (MHz)	75.48	***Nucleus***	13C	***Number of Transients***	1012	***Original Points Count***	16308
Points Count	16384	***Pulse Sequence***	zgpg30base	***Solvent***	CHLOROFORM-D	***Sweep Width (Hz)***	18115.94
Temperature (degree C)	22.100						



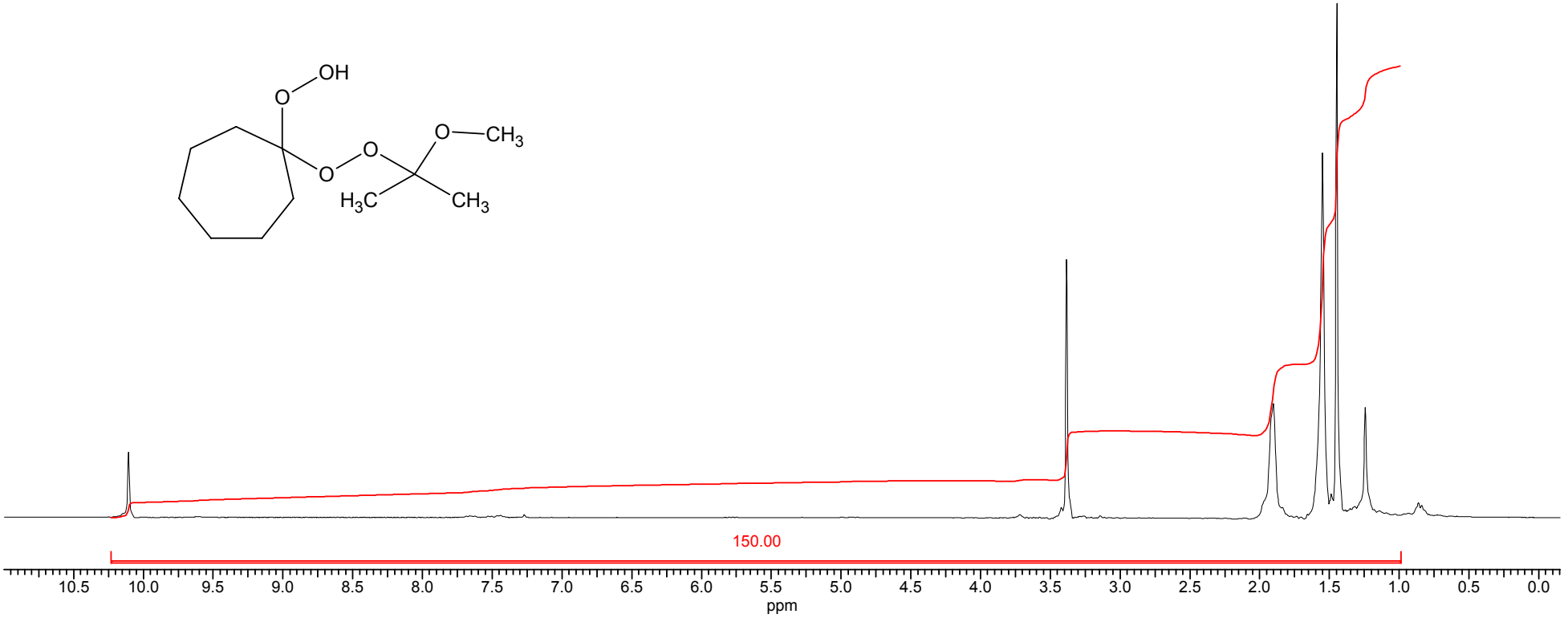
No.	(ppm)	(Hz)	Height
1	21.39	1614.1	0.1049
2	21.53	1625.2	0.3403
3	22.25	1679.4	0.3520
4	22.28	1681.6	1.0000
5	29.36	2215.7	0.8816
6	29.44	2222.3	0.2648
7	29.56	2231.2	0.3546
8	29.81	2250.0	0.4808
9	30.70	2317.4	0.7864
10	30.84	2327.4	0.1739
11	31.66	2389.3	0.1935

No.	(ppm)	(Hz)	Height
12	31.76	2397.0	0.3862
13	35.14	2652.5	0.2761
14	35.20	2656.9	0.4513
15	49.62	3745.0	0.1730
16	49.68	3749.4	0.2320
17	77.00	5811.7	0.2294
18	109.26	8246.6	0.1087
19	109.38	8255.4	0.2299
20	111.03	8380.4	0.0570
21	111.25	8397.0	0.2522

No.	Annotation	(ppm)
1	Chloroform-d	77.00

1-[(1-methoxy-1-methylethyl)peroxy]cycloheptyl hydroperoxide ***(5a)***

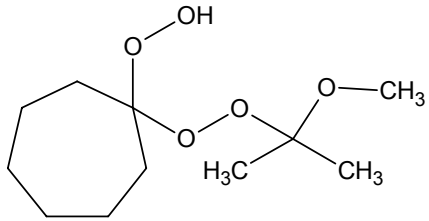
Acquisition Time (sec)	0.6759	***Date***	22 Feb 2008 10:57:04				
File Name	C:\Documents and Settings\Пользователь\Мои документы\Документы Платонов\Спектры фиды\plam\gemp178.{1H}\gemp178.{1H}_001000fid						
Frequency (MHz)	300.13	***Nucleus***	1H	***Number of Transients***	1	***Original Points Count***	8124
Points Count	8192	***Pulse Sequence***	zg	***Solvent***	CHLOROFORM-D	***Sweep Width (Hz)***	6009.62
Temperature (degree C)	35.200						



No.	(ppm)	Value
1	99 .. 10.2	150.000

1-[(1-methoxy-1-methylethyl)peroxy]cycloheptyl hydroperoxide ***(5a)***

Acquisition Time (sec)	0.3359	***Comment***	/PLAM GEMP178.C13 Opr:Struchkova M.I.;Solv:DMSO-d6;	***Date***	22/02/2008 16:07:23
File Name	C:\Documents and Settings\Пользователь\Мои документы\Документы Платонов\Спектры фиды\plam\gemp178.c13			***Frequency (MHz)***	50.32
Nucleus	13C	***Original Points Count***	8192	***Points Count*** 8192	***Solvent*** DMSO-D6
Sweep Width (Hz)	12195.12	***Temperature (degree C)***	24.000		

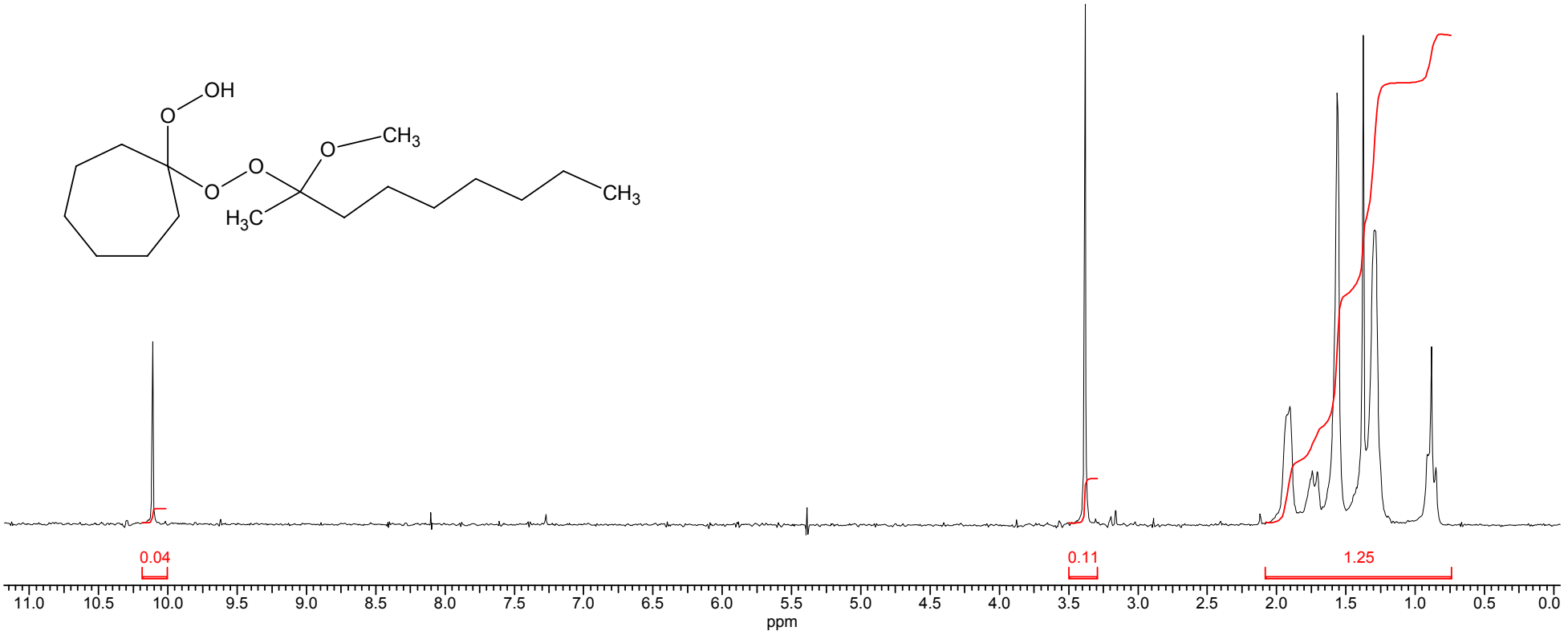


No.	(ppm)	(Hz)	Height
1	22.80	1147.3	0.9770
2	22.92	1153.3	1.0000
3	29.63	1491.3	0.1687
4	30.02	1510.6	0.7097
5	32.62	1641.6	0.7108
6	50.43	2537.9	0.3590
7	77.00	3874.9	0.1065
8	106.02	5335.5	0.1157
9	114.69	5771.7	0.1399

No.	Annotation	(ppm)
1	Chloroform-d	77.00

1-[(1-methoxy-1-methyloctyl)peroxy]cycloheptyl hydroperoxide ***(5b)***

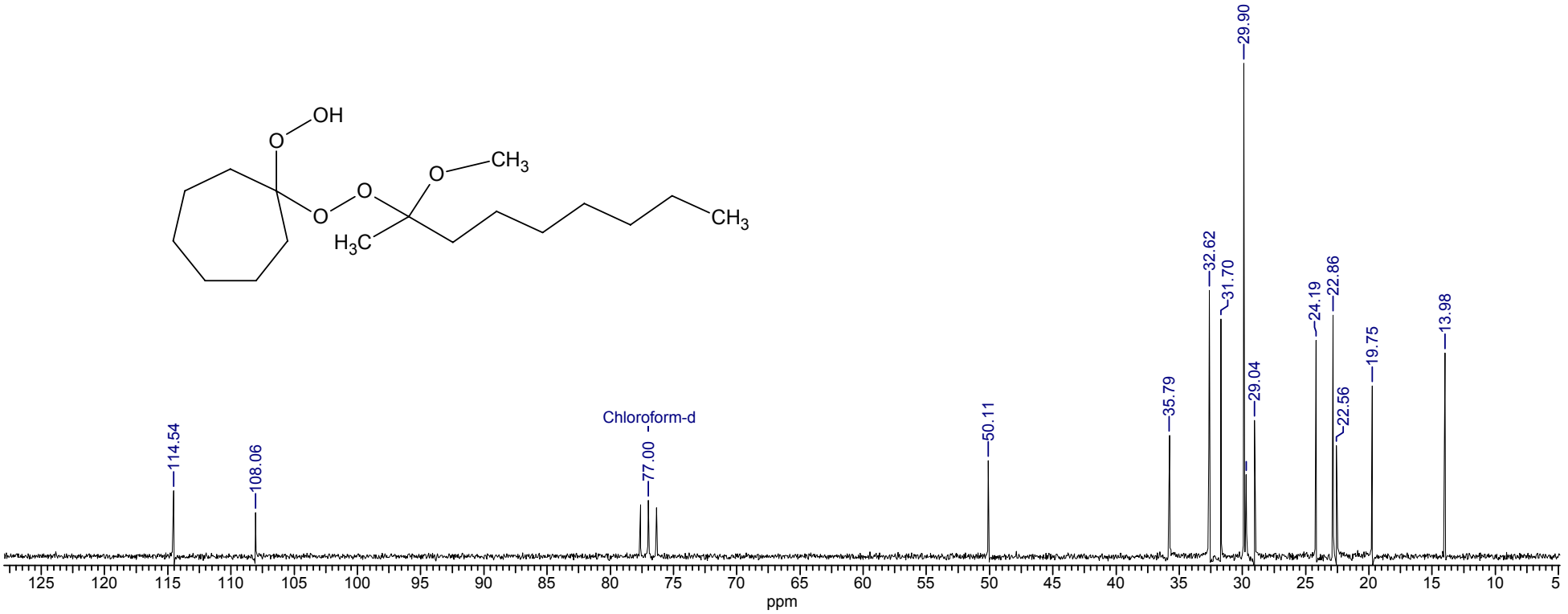
Acquisition Time (sec)	1.0240	***Comment***	/TERN IODID697□Opr:Struchkova M.I.;Solv:CDCl3;			***Date***	29/01/2008 17:54:26
File Name	C:\Documents and Settings\Пользователь\Мои документы\Документы Платонов\Спектры фиды\tern\iodid697					***Frequency (MHz)***	200.13
Nucleus	1H	***Number of Transients***	12	***Original Points Count***	8192	***Points Count***	8192
Solvent	DMSO-D6	***Sweep Width (Hz)***	4000.00	***Temperature (degree C)***	24.000		



No.	(ppm)	Value
1	.74 .. 2.0	1.252
2	.29 .. 3.5	0.114
3	.01 .. 10.	0.036

1-[(1-methoxy-1-methyloctyl)peroxy]cycloheptyl hydroperoxide ***(5b)***

Acquisition Time (sec)	0.3359	***Comment***	/TERN IODID697.C13□Opr:Struchkova M.I.;Solv:CDCl3;			***Date***	29/01/2008 19:26:33
File Name	C:\Documents and Settings\Пользователь\Мои документы\Документы Платонов\Спектры фиды\tern\iodid697.c13					***Frequency (MHz)***	50.32
Nucleus	13C	***Original Points Count***	8192	***Points Count***	8192	***Solvent***	DMSO-D6
Sweep Width (Hz)	12195.12	***Temperature (degree C)***	24.000				



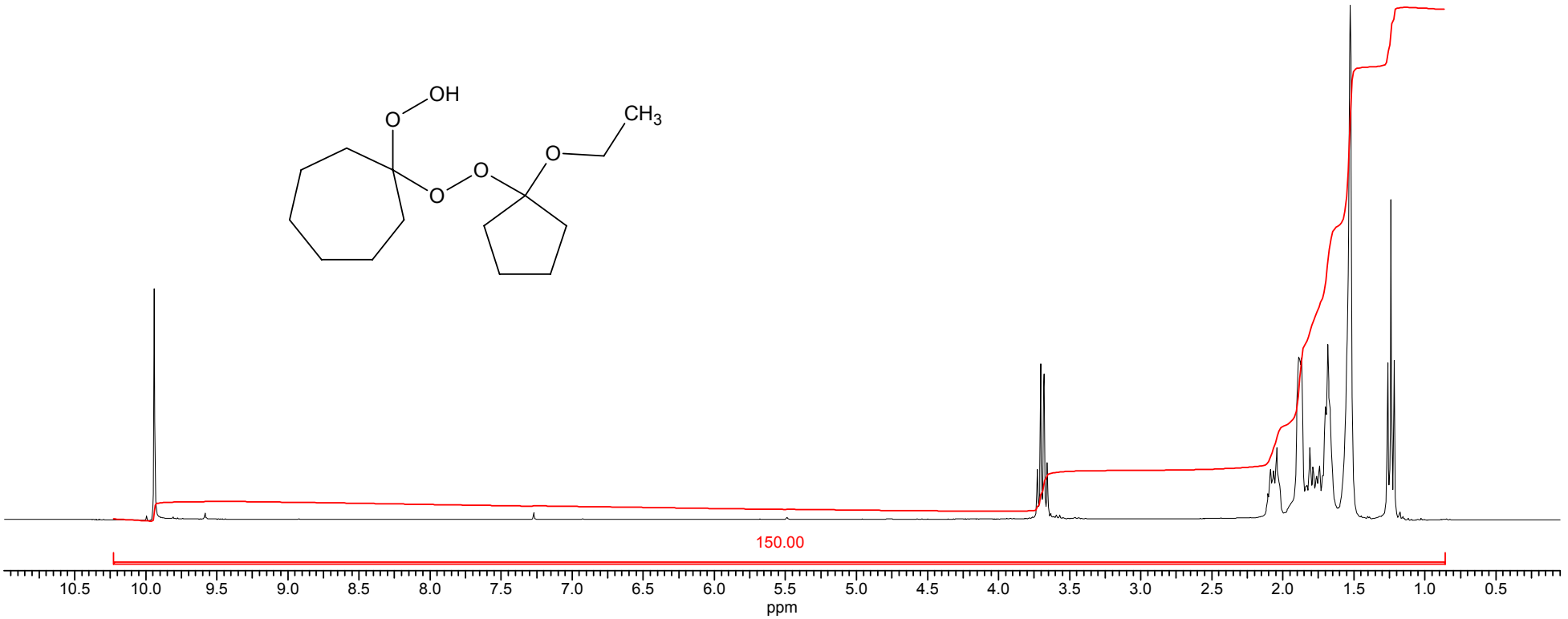
No.	(ppm)	(Hz)	Height
1	13.98	703.7	0.4124
2	19.75	994.0	0.3457
3	22.56	1135.4	0.2239
4	22.86	1150.3	0.4893
5	24.19	1217.3	0.4378
6	29.04	1461.5	0.2753
7	29.69	1494.2	0.1651
8	29.90	1504.7	1.0000

No.	(ppm)	(Hz)	Height
9	31.70	1595.5	0.4816
10	32.62	1641.6	0.5397
11	35.79	1800.9	0.2445
12	50.11	2521.5	0.1934
13	77.00	3874.9	0.1126
14	108.06	5438.2	0.0881
15	114.54	5764.2	0.1331

No.	Annotation	(ppm)
1	Chloroform-d	77.00

1-[(1-ethoxycyclopentyl)peroxy]cycloheptyl hydroperoxide ***(5c)***

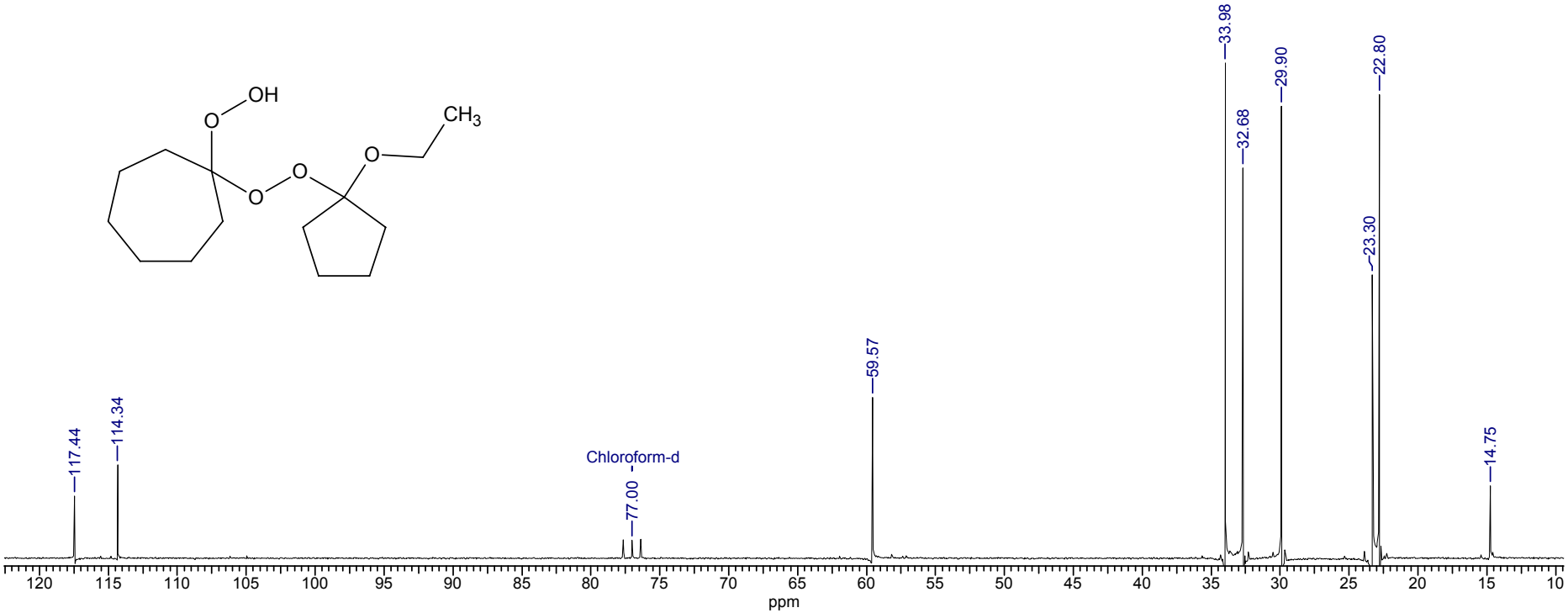
Acquisition Time (sec)	0.6759	***Comment***	Avance-300, CDCl3	***Date***	28 Jan 2008 14:49:36		
File Name	C:\Documents and Settings\Пользователь\Мои документы\Документы Платонов\Спектры фиды\tern\iodid707.001.{1H}\iodid707.001.{1H}_001000fid						
Frequency (MHz)	300.13	***Nucleus***	1H	***Number of Transients***	1	***Original Points Count***	8124
Points Count	8192	***Pulse Sequence***	zg	***Solvent***	CHLOROFORM-D	***Sweep Width (Hz)***	6009.62
Temperature (degree C)	30.000						



No.	(ppm)	Value
1	86 .. 10.2	150.000

1-[(1-ethoxycyclopentyl)peroxy]cycloheptyl hydroperoxide ***(5c)***

Acquisition Time (sec)	0.3359	***Comment***	/TERN IODID707.C13□Opr:Struchkova M.I.;Solv:CDCl3;	***Date***	29/01/2008 19:04:31
File Name	C:\Documents and Settings\Пользователь\Мои документы\Документы Платонов\Спектры фиды\tern\iodid707.c13			***Frequency (MHz)***	50.32
Nucleus	13C	***Original Points Count***	8192	***Solvent***	DMSO-D6
Sweep Width (Hz)	12195.12	***Temperature (degree C)***	24.000		

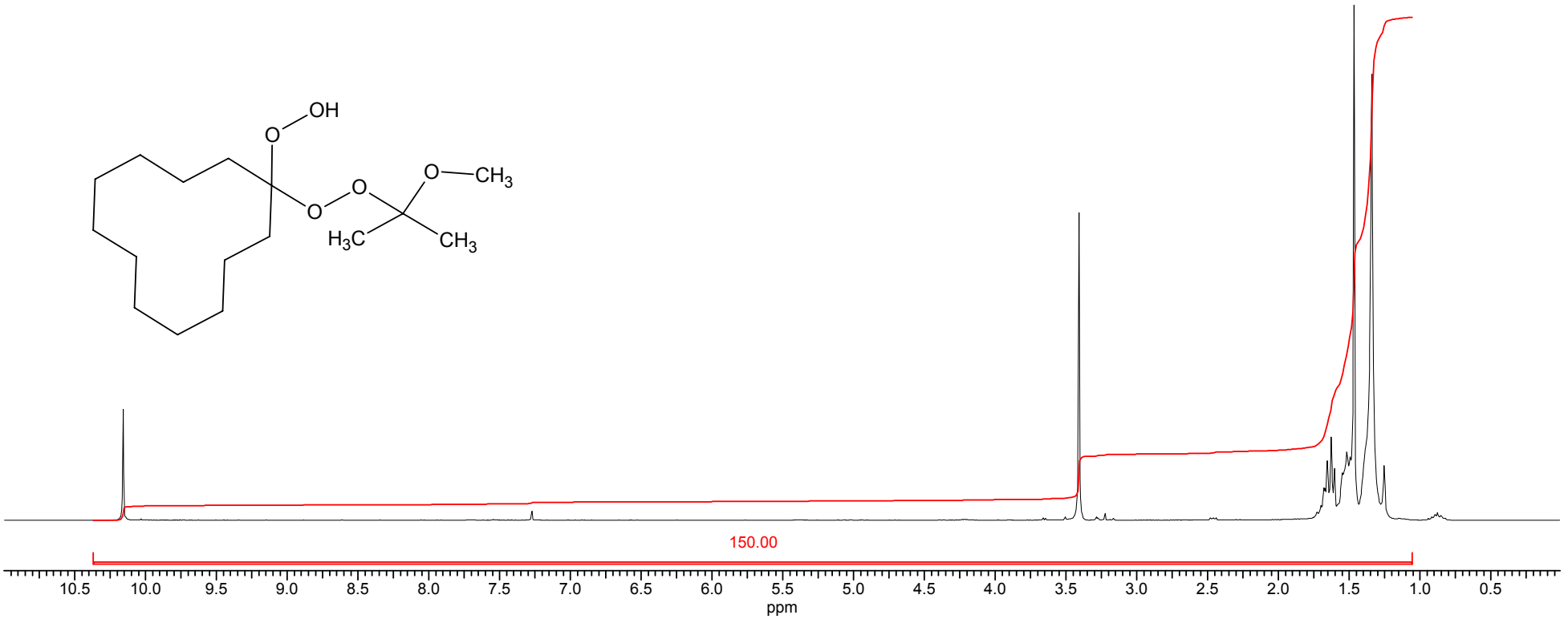


No.	(ppm)	(Hz)	Height
1	14.75	742.4	0.1458
2	22.80	1147.4	0.9364
3	23.30	1172.7	0.5719
4	29.90	1504.7	0.9123
5	32.68	1644.6	0.7876
6	33.98	1710.2	1.0000
7	59.57	2998.0	0.3241
8	77.00	3874.9	0.0356
9	114.34	5753.9	0.1876
10	117.44	5910.2	0.1246

No.	Annotation	(ppm)
1	Chloroform-d	77.00

1-[(1-methoxy-1-methylethyl)peroxy]cyclododecyl hydroperoxide ***(6a)***

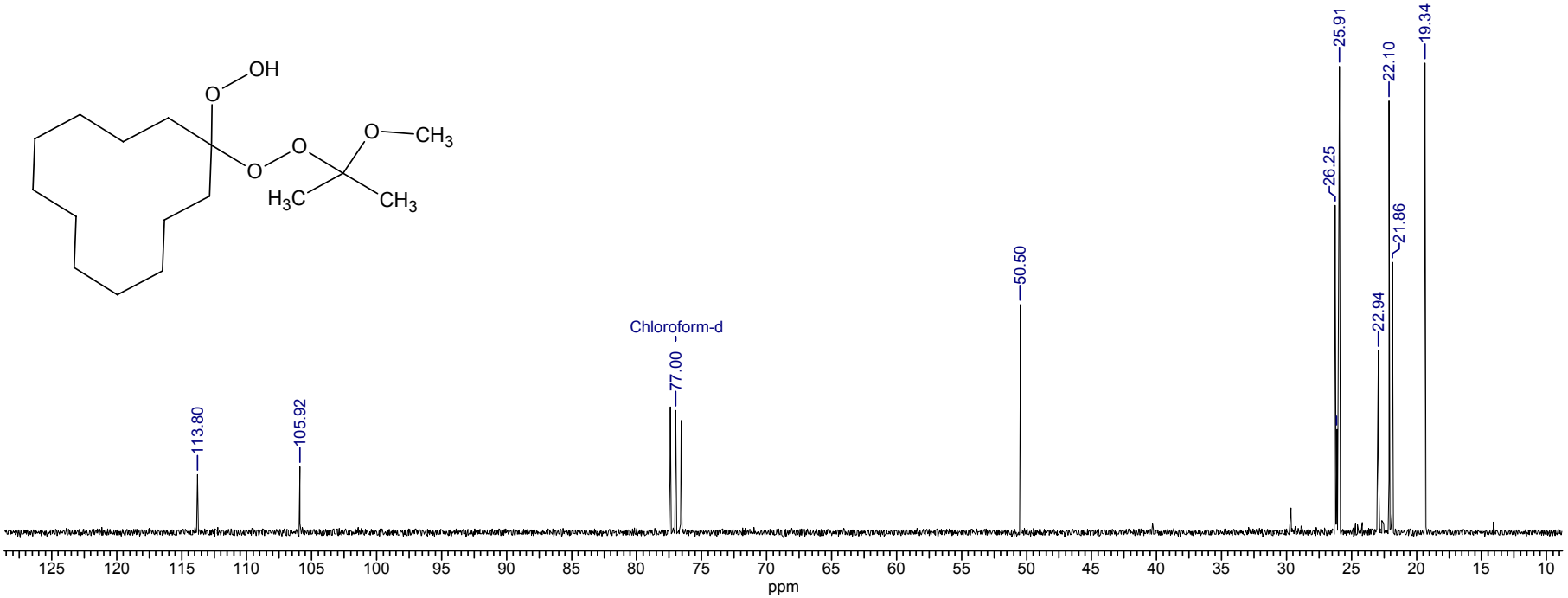
Acquisition Time (sec)	0.6759	***Comment***	Avance-300, CDCl3	***Date***	23 Jan 2008 10:44:16		
File Name	C:\Documents and Settings\Пользователь\Мои документы\Документы Платонов\Спектры фиды\plam\gemp166.001.{1H}\gemp166.001.{1H}_001000fid						
Frequency (MHz)	300.13	***Nucleus***	1H	***Number of Transients***	1	***Original Points Count***	8124
Points Count	8192	***Pulse Sequence***	zg	***Solvent***	CHLOROFORM-D	***Sweep Width (Hz)***	6009.62
Temperature (degree C)	21.700						



No.	(ppm)	Value
1	05 .. 10.3	150.000

1-[(1-methoxy-1-methylethyl)peroxy]cyclododecyl hydroperoxide ***(6a)***

Acquisition Time (sec)	0.4501	***Comment***	Avance-300, C-13, CDCl3			***Date***	23 Jan 2008 10:46:24
File Name	C:\Documents and Settings\Пользователь\Мои документы\Документы Платонов\Спектры фиды\plam\gemp166.013.{13C}\gemp166.013.{13C}_013000fid						
Frequency (MHz)	75.48	***Nucleus***	13C	***Number of Transients***	623	***Original Points Count***	16308
Points Count	16384	***Pulse Sequence***	zgpg30base	***Solvent***	CHLOROFORM-D	***Sweep Width (Hz)***	18115.94
Temperature (degree C)	21.800						

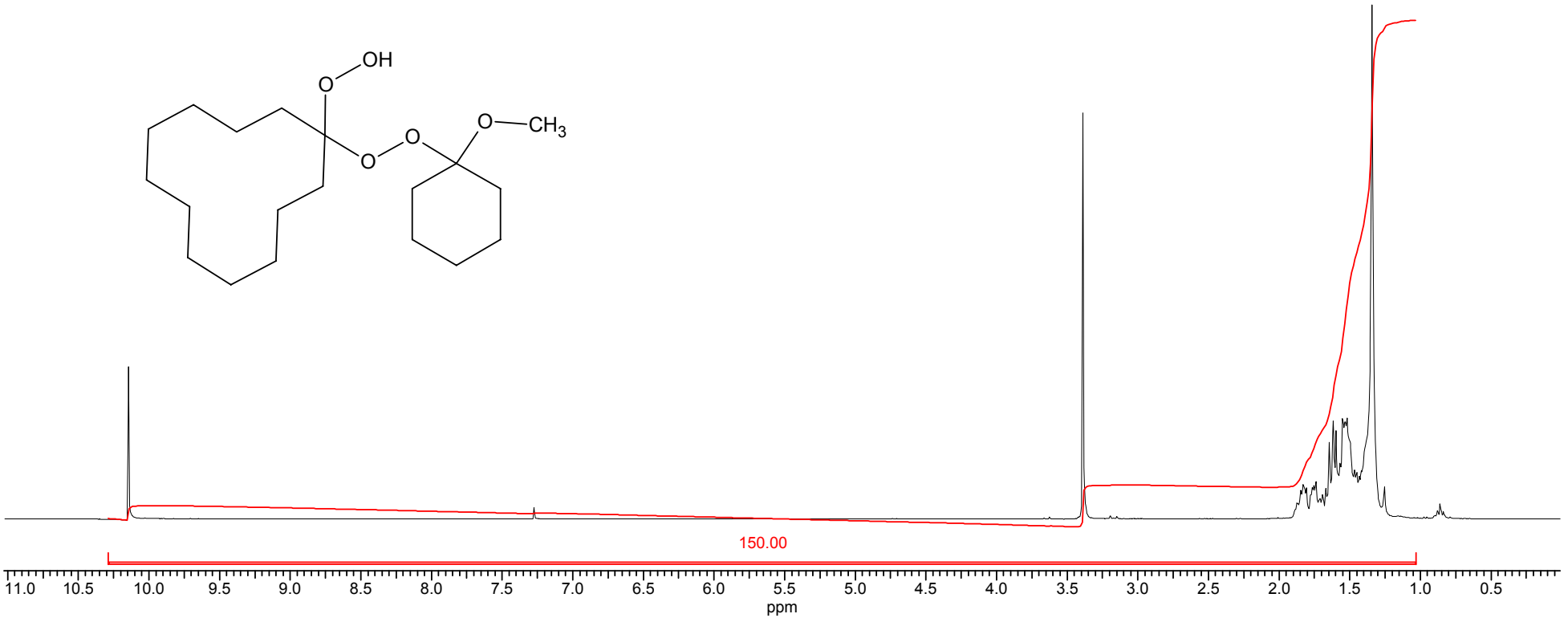


No.	(ppm)	(Hz)	Height
1	19.34	1459.3	1.0000
2	21.86	1649.5	0.5766
3	22.10	1668.3	0.9195
4	22.94	1731.4	0.3873
5	25.91	1955.8	0.9933
6	26.13	1972.4	0.2205
7	26.25	1981.3	0.6974
8	50.50	3811.3	0.4864
9	77.00	5811.7	0.2602
10	105.92	7994.5	0.1400
11	113.80	8589.4	0.1234

No.	Annotation	(ppm)
1	Chloroform-d	77.00

1-[(1-methoxycyclohexyl)peroxy]cyclododecyl hydroperoxide ***(6d)***

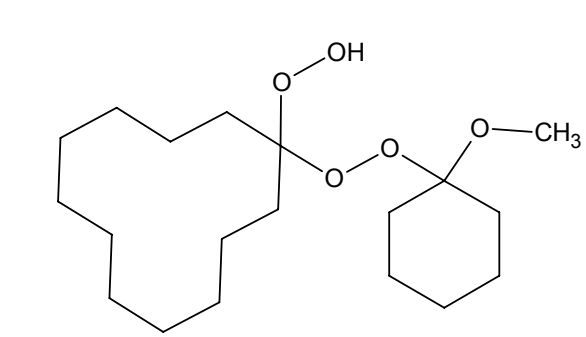
Acquisition Time (sec)	0.6759	***Comment***	Avance-300, CDCl3	***Date***	29 Jan 2008 14:26:08		
File Name	C:\Documents and Settings\Пользователь\Мои документы\Документы Платонов\Спектры фиды\plam\gemp171.001.{1H}\gemp171.001.{1H}_001000fid						
Frequency (MHz)	300.13	***Nucleus***	1H	***Number of Transients***	1	***Original Points Count***	8124
Points Count	8192	***Pulse Sequence***	zg	***Solvent***	CHLOROFORM-D	***Sweep Width (Hz)***	6009.62
Temperature (degree C)	22.500						



No.	(ppm)	Value
1	03 .. 10.2	150.000

1-[(1-methoxycyclohexyl)peroxy]cyclododecyl hydroperoxide ***(6d)***

Acquisition Time (sec)	0.4501	***Comment***	Avance-300, C-13, CDCl3			***Date***	29 Jan 2008 14:26:08
File Name	C:\Documents and Settings\Пользователь\Мои документы\Документы Платонов\Спектры фиды\plam\gemp171.013.{13C}\gemp171.013.{13C}_013000fid						
Frequency (MHz)	75.48	***Nucleus***	13C	***Number of Transients***	528	***Original Points Count***	16308
Points Count	16384	***Pulse Sequence***	zgpg30base	***Solvent***	CHLOROFORM-D	***Sweep Width (Hz)***	18115.94
Temperature (degree C)	22.500						



No.	(ppm)	(Hz)	Height
1	19.33	1459.3	0.4048
2	21.84	1648.4	0.5933
3	22.07	1666.1	0.7844
4	22.79	1720.3	0.5657
5	25.31	1910.5	0.3220
6	25.90	1954.7	1.0000
7	26.15	1973.5	0.3431

No.	(ppm)	(Hz)	Height
8	26.24	1980.1	0.7832
9	31.73	2394.8	0.3427
10	49.37	3726.1	0.3409
11	77.00	5811.6	0.1700
12	106.17	8013.2	0.2573
13	113.52	8568.3	0.1859

No.	Annotation	(ppm)
1	Chloroform-d	77.00