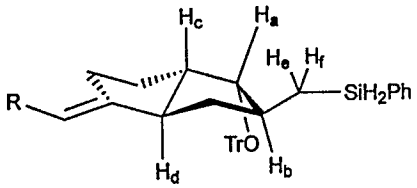
JOC The Journal of Organic Chemistry

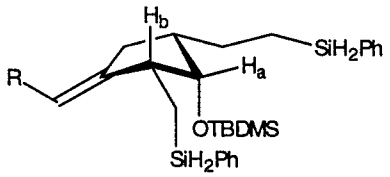
J. Org. Chem., 1998, 63(16), 5507-5516, DOI:10.1021/jo980521t

exp5 ro2pulnoe

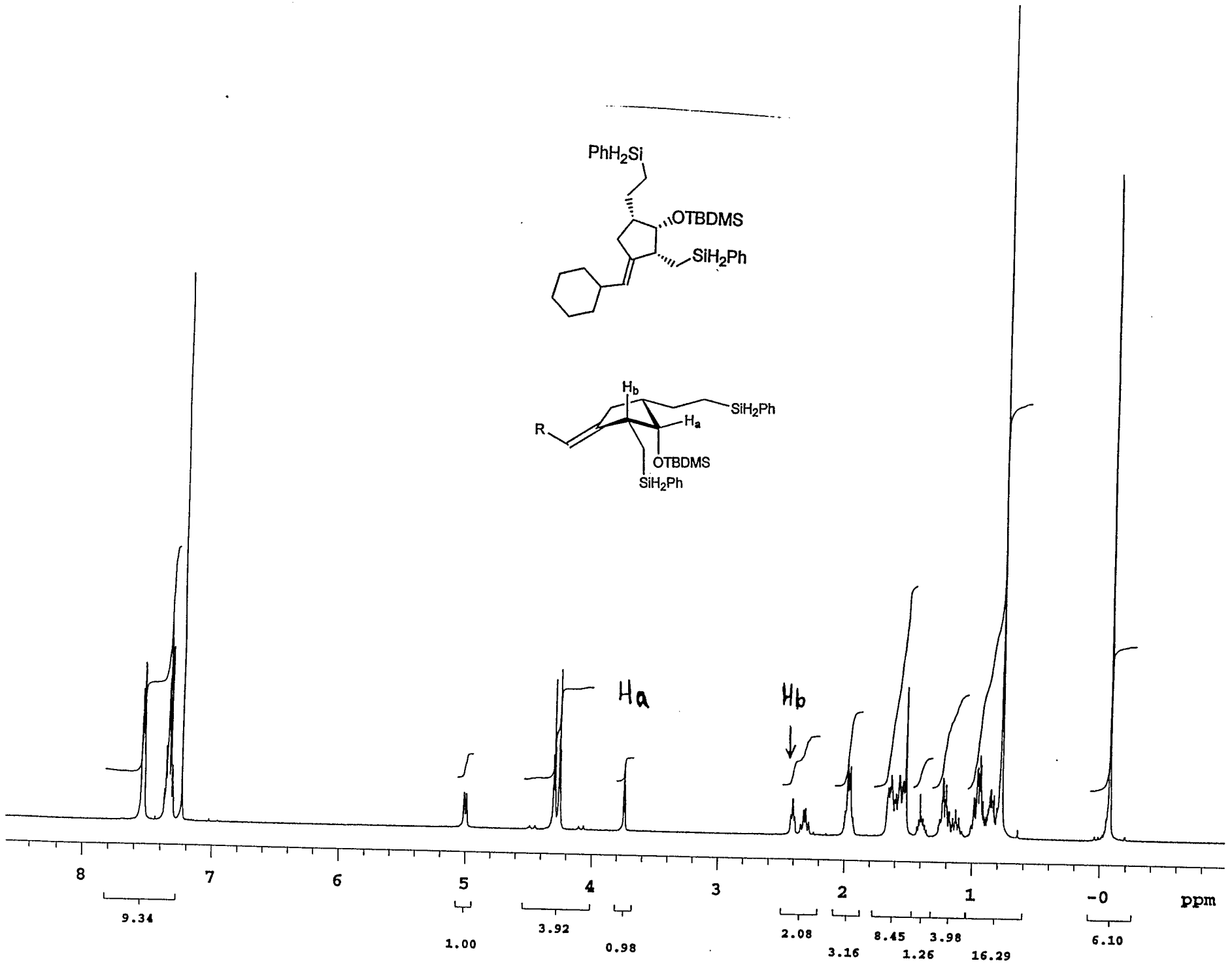
SAMPLE		DEC. & VT		ACQUISITION ARRAYS	
date	Oct 4 97	dn	H1	array	dof
solvent	CDCl3	dof	arrayed	arraydim	4
file	/nmrdata/rgro~	dm	nyn		
ups/molander/bill/~	br714noe	dmm	c	i	dof
		dmf	200	1	-633
ACQUISITION		dpwr	-6	2	-1008.4
sfrq	500.370	PROCESSING		3	-1420.3
tn	H1	lb	1.00	4	2017.5
at	5.043	fn	not used		
np	100928	math	i		
sw	10007.5				
fb	6000	werr	react		
bs	16	wexp	wft		
ss	8	wbs			
pw	13.5	wnt			
pw	13.5	DISPLAY			
tpwr	58	sp	-107.9		
d1	3.000	wp	4213.6		
tof	273.7	vs	19534		
nt	1024	sc	0		
ct	1024	wc	250		
alock	n	hzmm	16.85		
gain	40	is	128000.00		
FLAGS		rf1	5872.4		
il	y	rfp	3622.7		
in	y	th	20		
dp	y	ins	70.698		
hs	nn	ai	ph		



NOE Data for **61**.



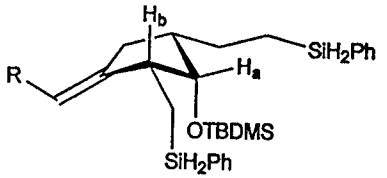
H_a	H_b
ir.	4.8%

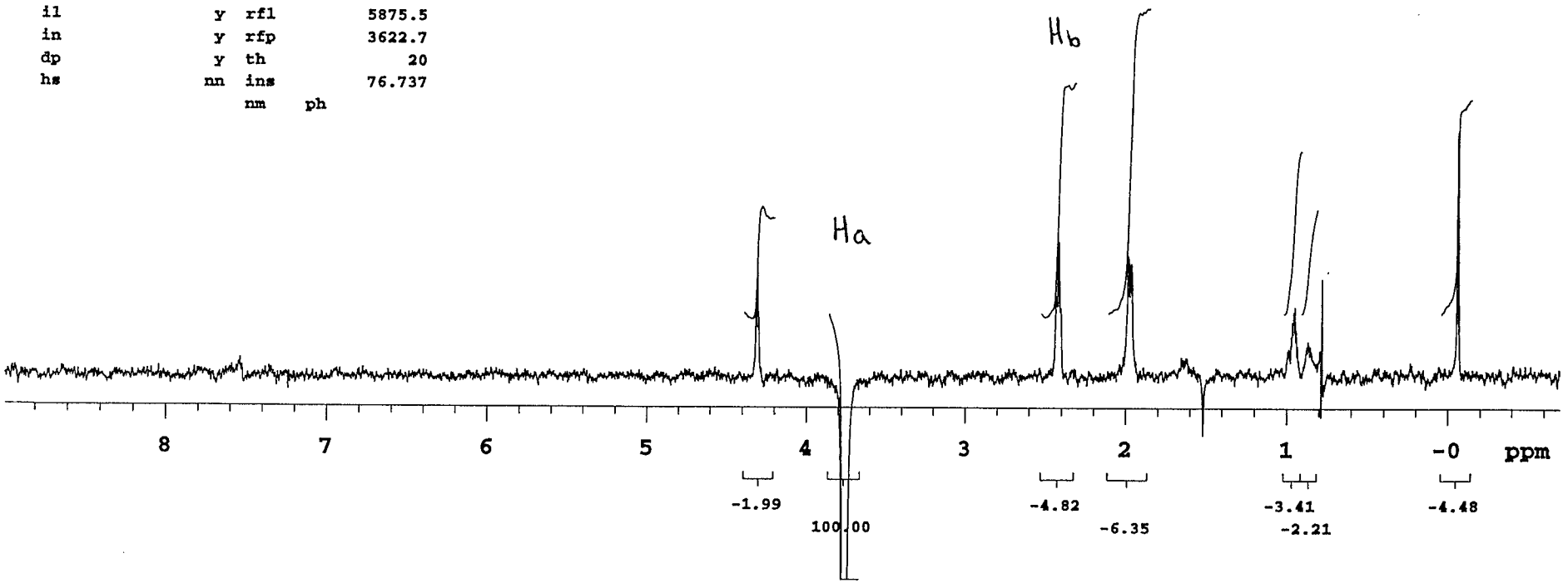


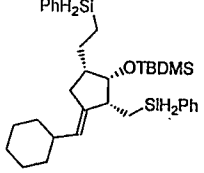
new experiment

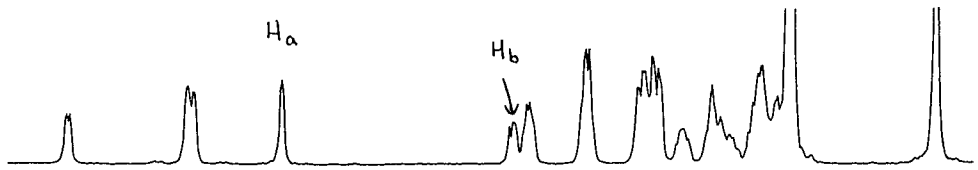
exp5 ro2pulnoe

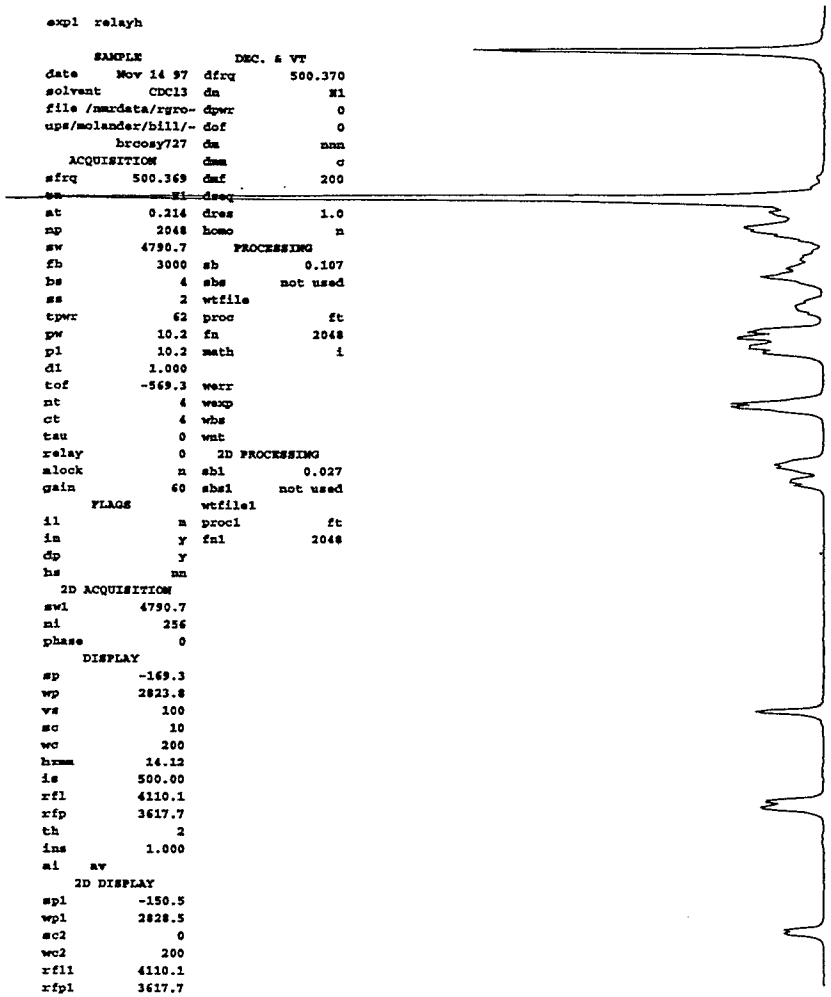
SAMPLE		DEC. & VT		ACQUISITION ARRAYS	
date	Nov 14 97	dn	H1	array	dof
solvent	CDCl3	dof	arrayed	arraydim	2
file	/nmrdata/rgro~	dm	nyn		
ups/molander/bill/~		dmm	c	i	dof
	br727noe	dmf	200	1	-600.1
ACQUISITION		dpwr	-6	2	2251.4
sfrq	500.370	temp	25.0		
tn	H1	PROCESSING			
at	5.043	lb	1.00		
np	100928	fn	not used		
sw	10007.5	math	i		
fb	6000				
bs	4	werr	react		
ss	8	wexp	wft		
pw	13.5	wbs			
pw	13.5	wnt			
tpwr	58	DISPLAY			
d1	3.000	sp	-350.8		
tof	273.7	wp	4841.5		
nt	128	vs	771		
ct	128	sc	0		
alock	n	wc	250		
gain	30	hzmm	19.37		
FLAGS		is	1.73336e+06		
il	y	rfl	5875.5		
in	y	rfp	3622.7		
dp	y	th	20		
hs	nn	ins	76.737		
		nm	ph		



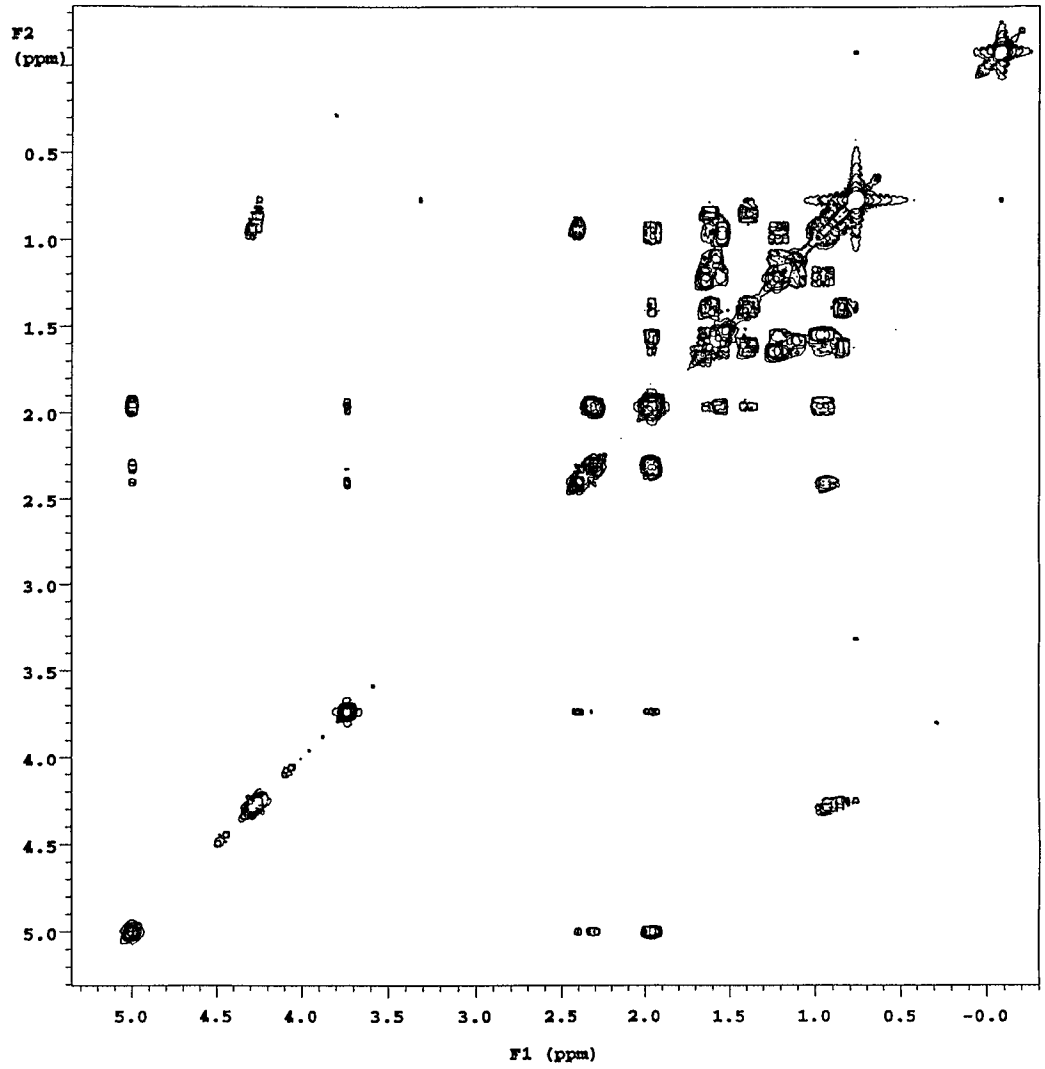




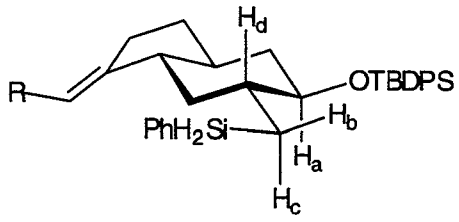




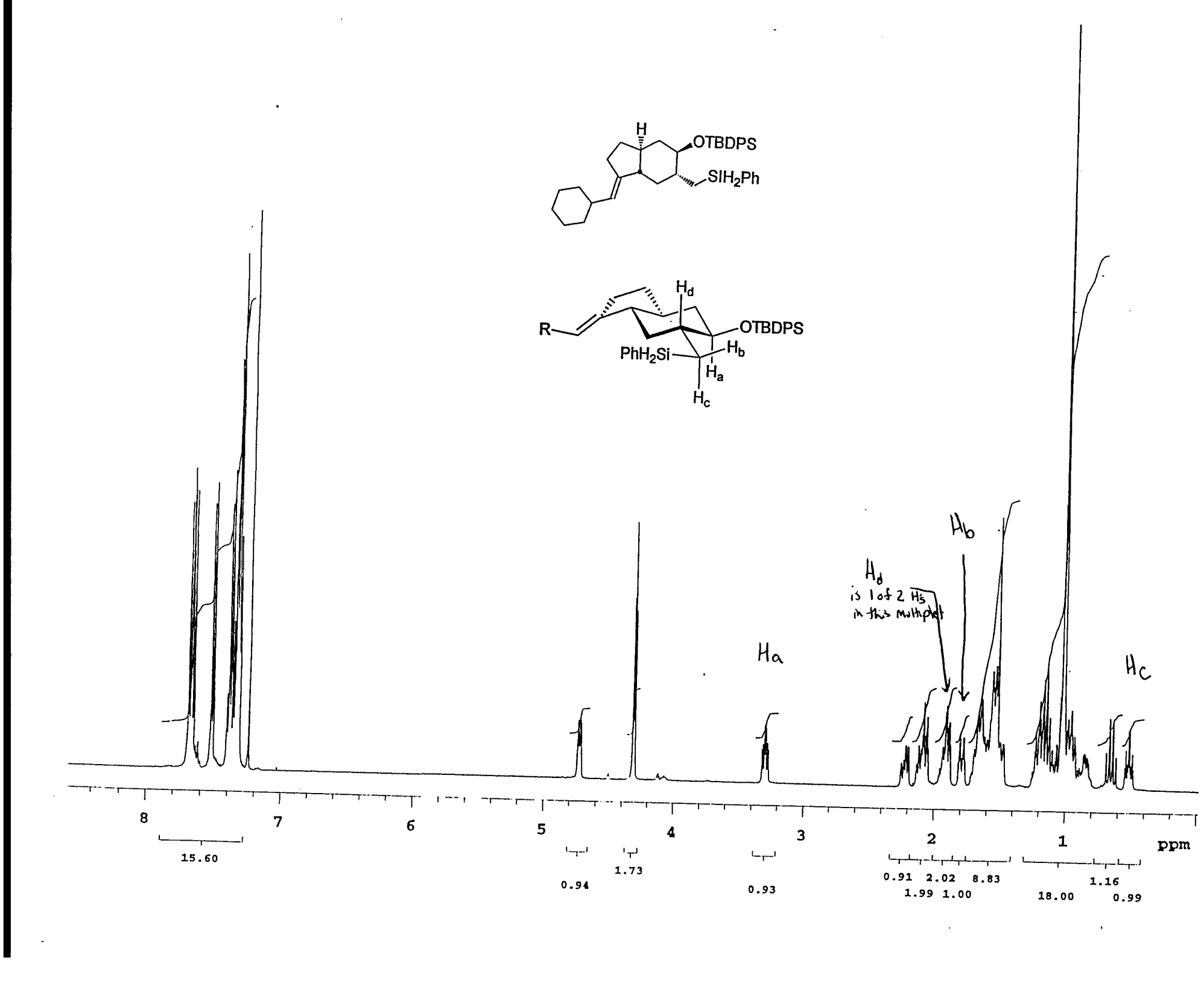
```
expl  relayh

      SAMPLE                DEC. & VT
date      Nov 14 97   dfrq        500.370
solvent       CDCl3   dn             H1
file /nmrdata/rgro-   dpwr              0
ups/molander/bill/-   dof               0
          hrcosy727   dm              nnn
   ACQUISITION        dmm               c
sfrq        500.369   dmf             200
tn             H1     dseq
at           0.214   dres            1.0
np            2048   homo              n
sw          4790.7       PROCESSING
fb            3000   sb            0.107
bs               4   sbs       not used
ss               2   wtfile
tpwr            62   proc             ft
pw            10.2   fn             2048
p1            10.2   math              i
d1           1.000
tof         -569.3   werr
nt               4   wexp
ct               4   wbs
tau              0   wnt
relay            0     2D PROCESSING
alock            n   sb1           0.027
gain            60   sbs1      not used
      FLAGS          wtfile1
il               n   proc1            ft
in               y   fn1            2048
dp               y
hs              nn
  2D ACQUISITION
sw1         4790.7
ni             256
phase            0
     DISPLAY
sp          -169.3
wp          2823.8
vs             100
sc              10
wc             200
hzmm         14.12
is          500.00
rfl         4110.1
rfp         3617.7
th               2
ins          1.000
ai    av
   2D DISPLAY
sp1         -150.5
wp1         2828.5
sc2              0
wc2            200
rf11        4110.1
rfp1        3617.7
```

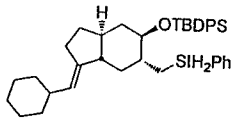


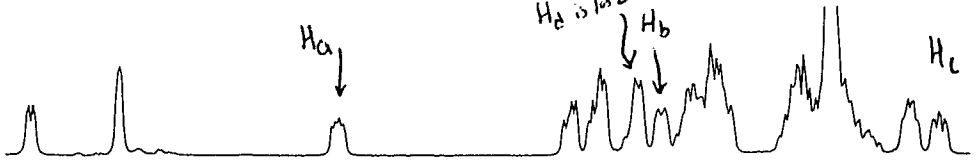
NOE Data for **62**.

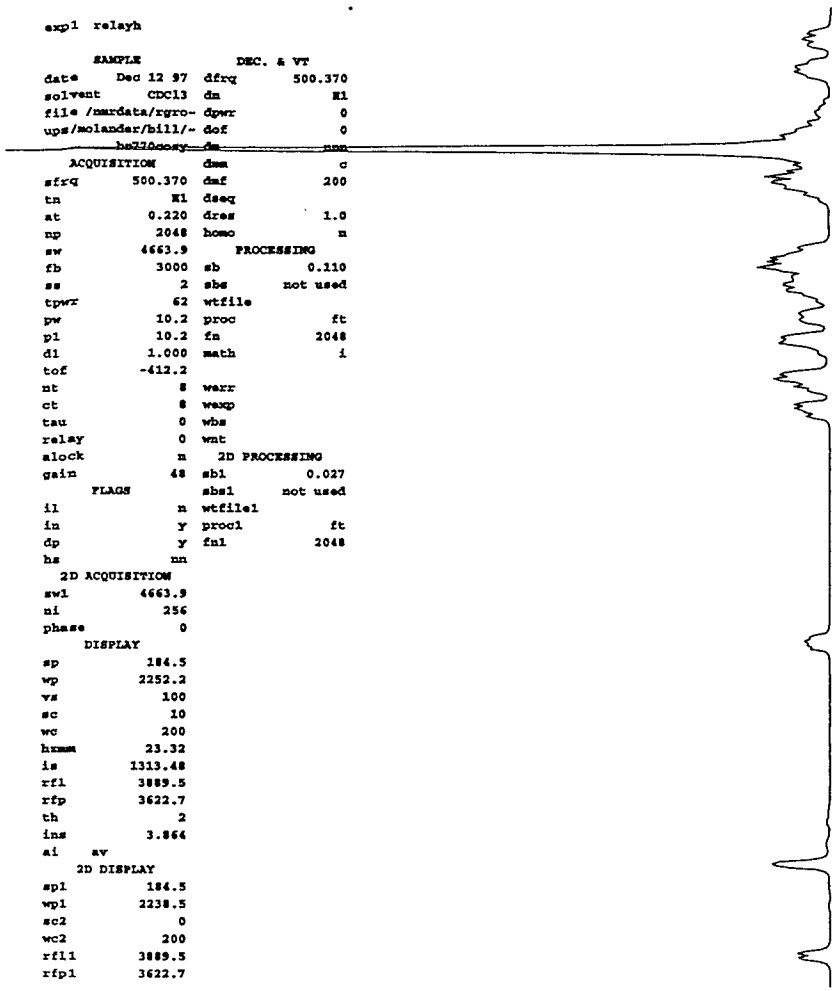


H_a	H_b	H_c	H_d
ir.	2.8%	4.3%	0%

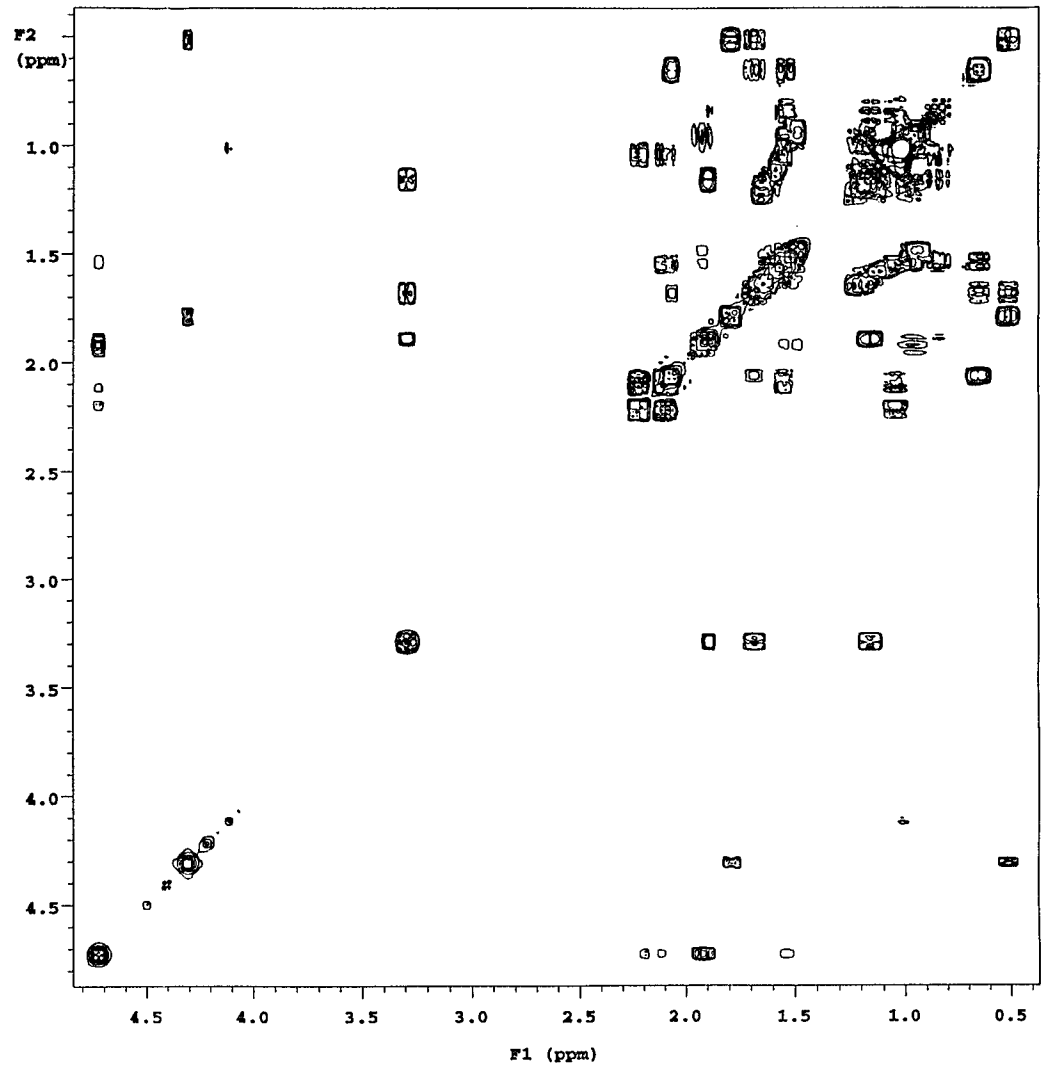








```
exp1  relayh

      SAMPLE              DEC. & VT
date      Dec 12 97   dfrq        500.370
solvent       CDCl3   dn               H1
file /nmrdata/rgro-   dpwr              0
ups/molander/bill/~   dof               0
        hs270cosy     dm              nnn
   ACQUISITION        dmm               c
sfrq        500.370   dmf             200
tn               H1   dseq
at            0.220   dres            1.0
np             2048   homo              n
sw           4663.9      PROCESSING
fb             3000   sb            0.110
ss                2   sbs         not used
tpwr             62   wtfile
pw             10.2   proc              ft
pl             10.2   fn              2048
d1            1.000   math               i
tof          -412.2
nt                8   werr
ct                8   wexp
tau               0   wbs
relay             0   wnt
alock             n     2D PROCESSING
gain             48   sb1           0.027
      FLAGS           sbs1        not used
il                n   wtfile1
in                y   proc1             ft
dp                y   fn1             2048
hs               nn
  2D ACQUISITION
sw1          4663.9
ni              256
phase             0
     DISPLAY
sp            184.5
wp           2252.2
vs              100
sc               10
wc              200
hzmm          23.32
is          1313.48
rf1          3889.5
rfp          3622.7
th                2
ins           3.864
ai    av
    2D DISPLAY
sp1           184.5
wp1          2238.5
sc2               0
wc2             200
rf11         3889.5
rfp1         3622.7
```



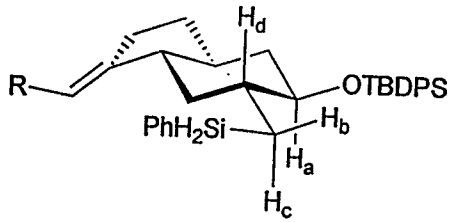
new experiment

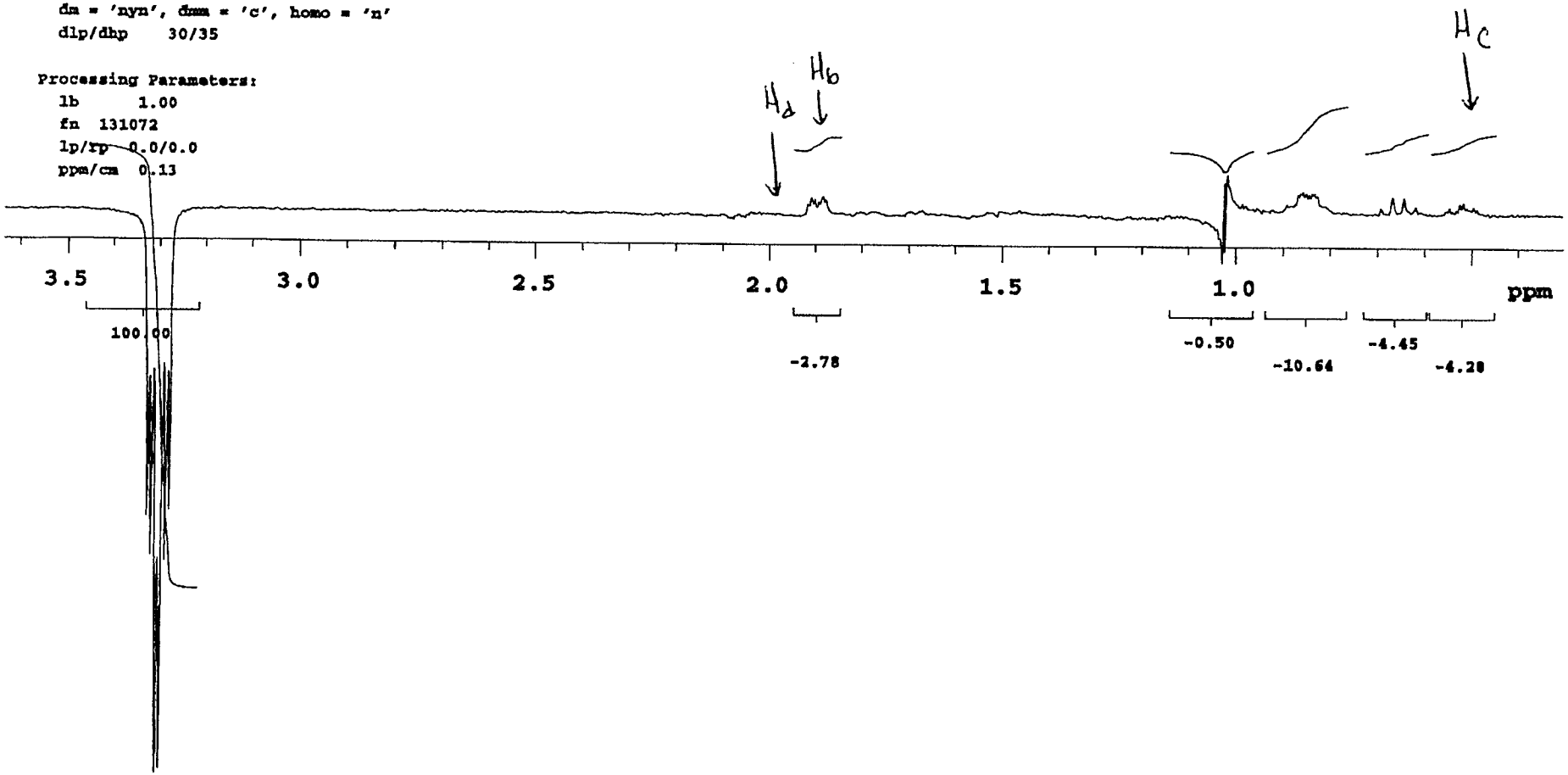
File: billnoe.1 (Varian Data)
Date: Dec 20 97

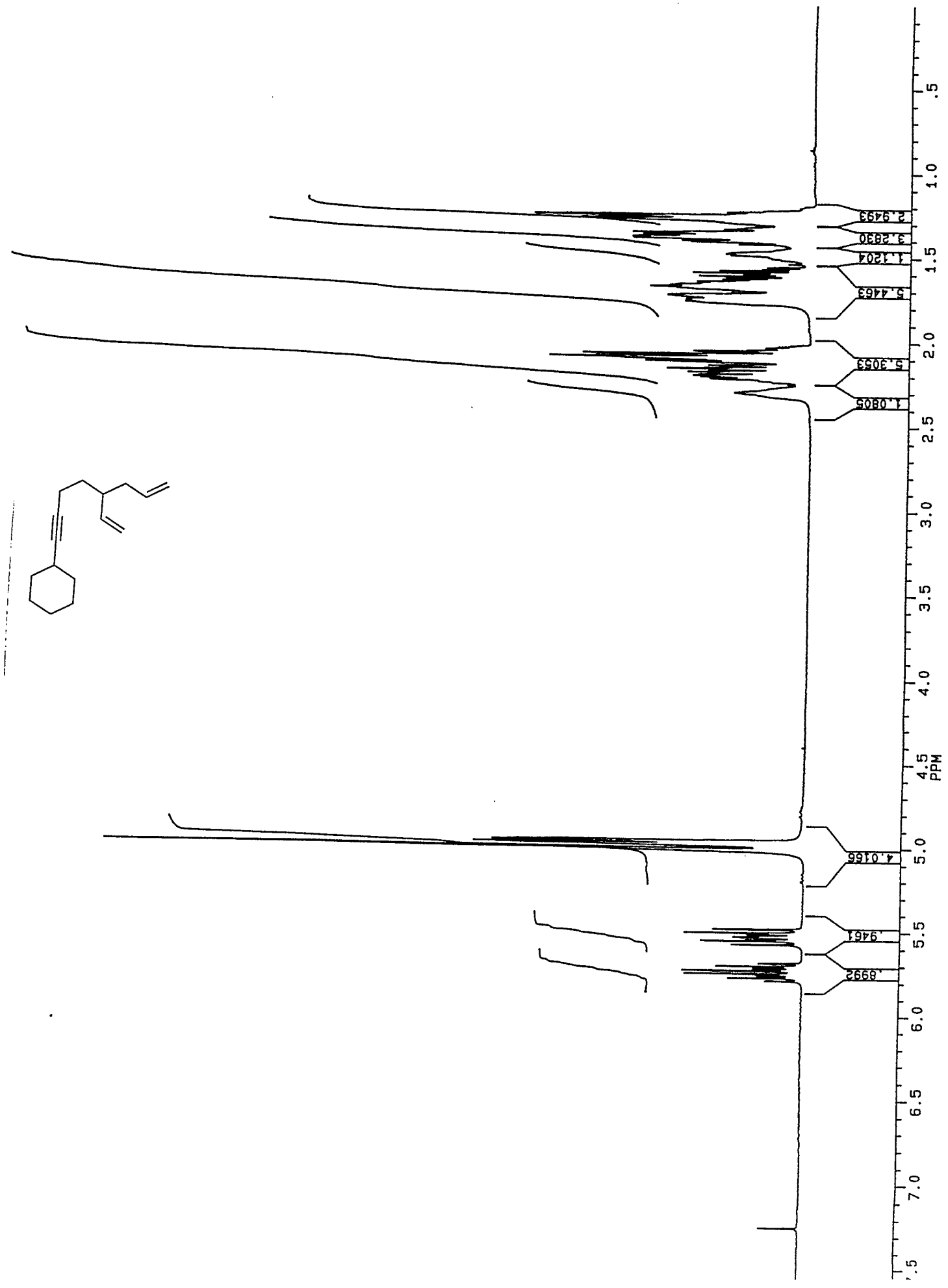
Acquisition Parameters:
Nucleus: H1 at 500.370 MHz
Solvent: CDCl3
tof 273.7
sw 6504.6 Hz (13.000 ppm)
pw 10.25 usec
d1 15.000 sec
np 65600
at 5.043 sec
bs/ss 8/4
nt/ct 64/64

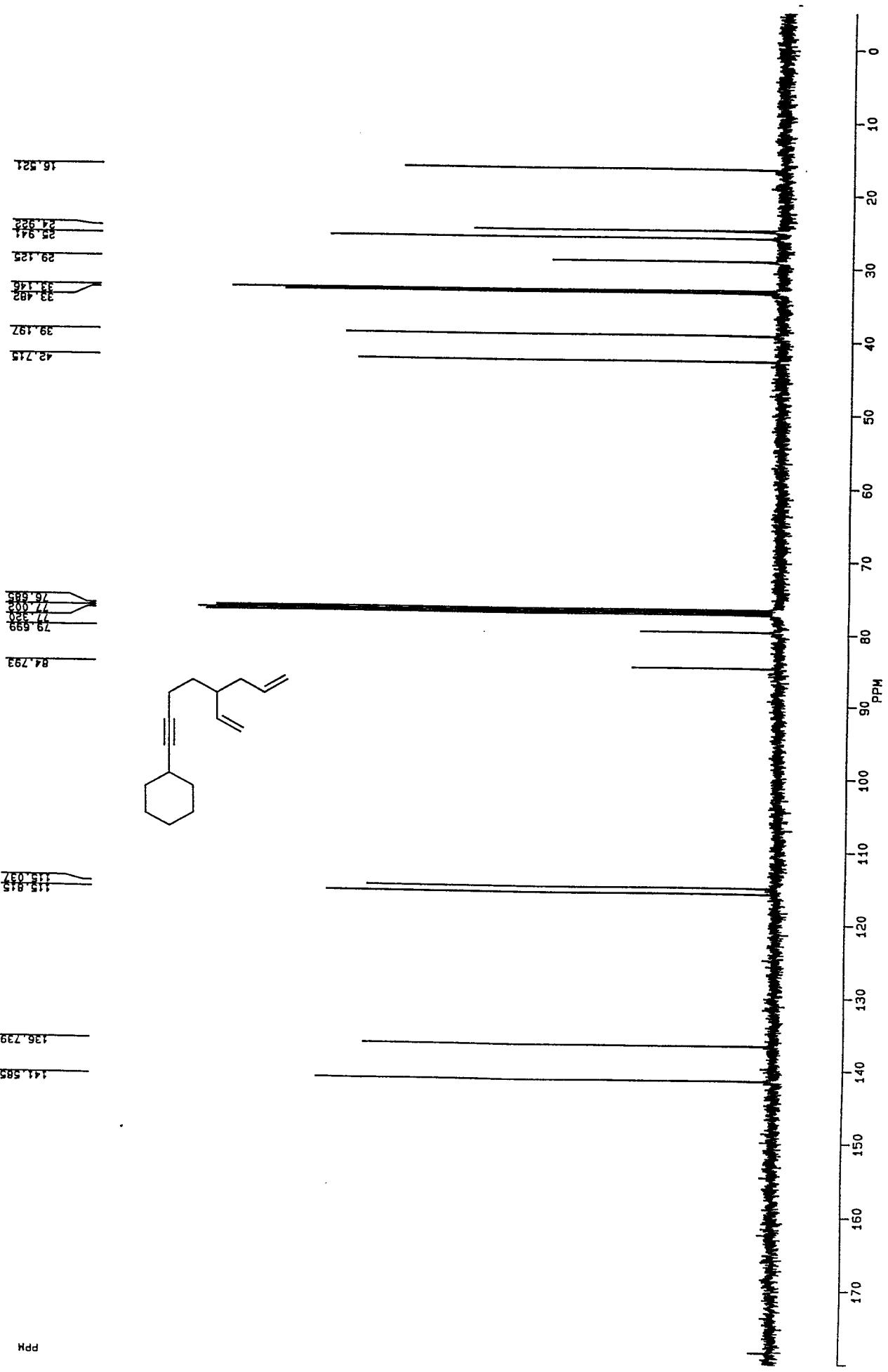
Decoupling Parameters:
Nucleus: H1, dof: -824.8
dm = 'nyn', dmm = 'c', homo = 'n'
dlp/dhp 30/35

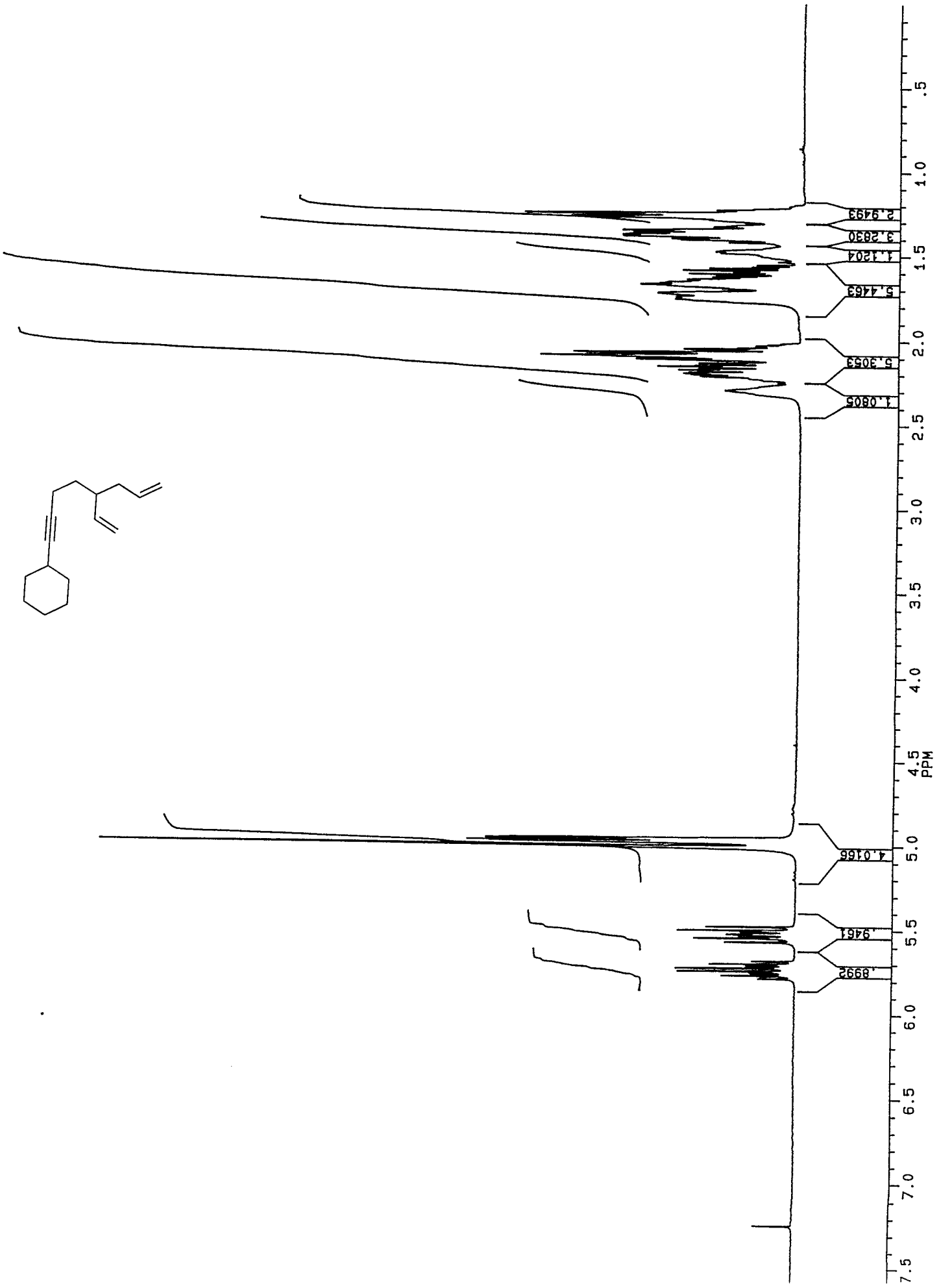
Processing Parameters:
lb 1.00
fn 131072
lp/rp 0.0/0.0
ppm/cm 0.13

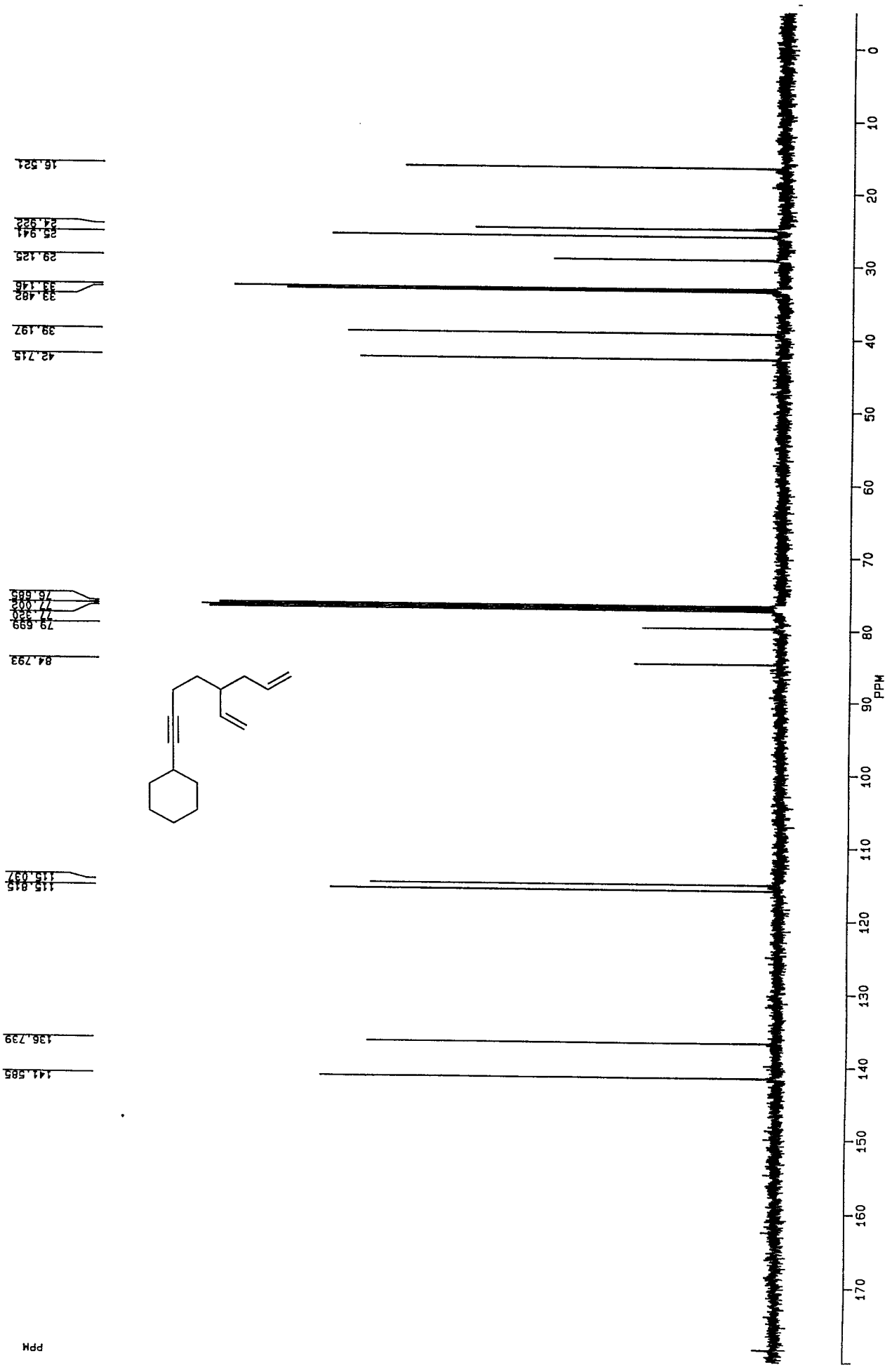


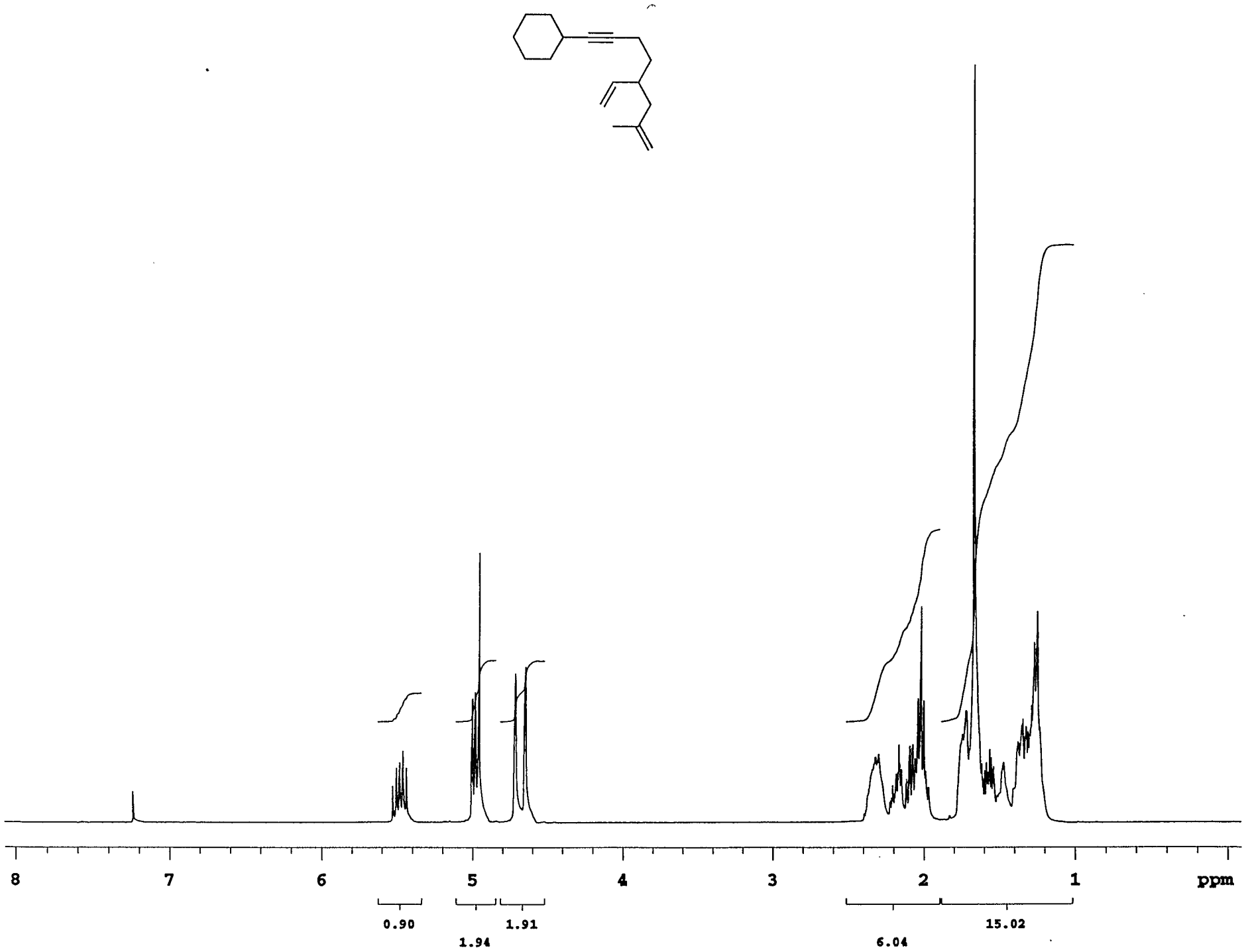



2.9493
3.2830
1.1204
5.4463
5.3053
1.0805
4.0166
.9461
.8992
PPM
.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5

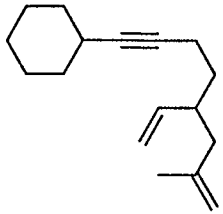

16.521
24.922
25.941
29.125
33.146
33.482
39.192
42.715
76.685
77.002
77.320
79.699
84.793
115.037
115.815
136.739
141.585
PPM
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
PPM

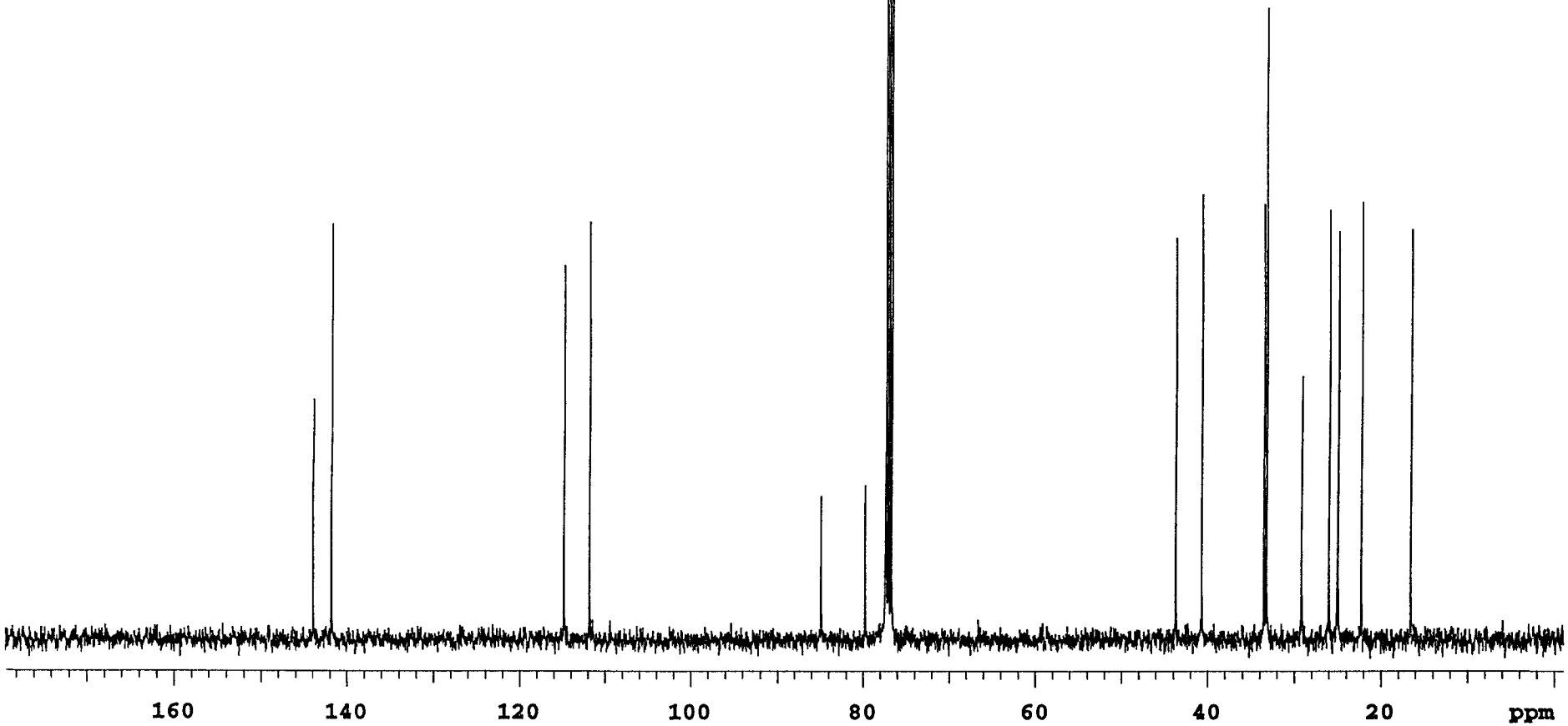

2.9493
3.2830
1.1204
5.4463
5.3053
1.0805
4.0166
.9461
.8992
.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
PPM
5.0
5.5
6.0
6.5
7.0
7.5

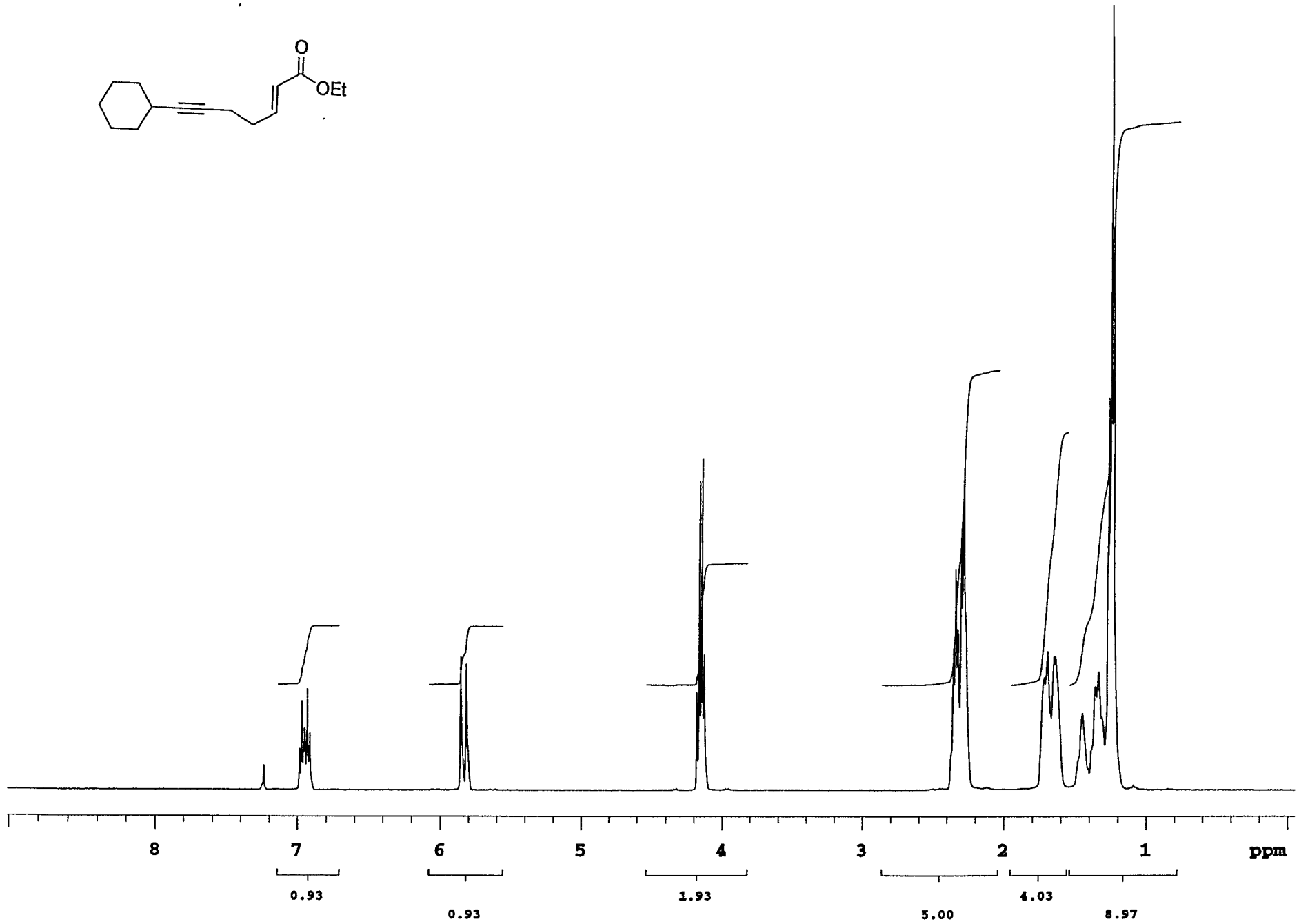

16.521
24.922
25.941
29.125
33.148
33.482
39.192
42.715
76.865
77.192
77.305
77.320
79.699
84.793
115.097
115.815
136.739
141.585
PPM
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
PPM



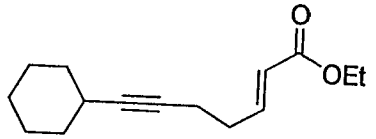
INDEX	FREQUENCY	PPM	HEIGHT
1	14476.181	143.873	0.9
2	14266.911	141.793	1.5
3	11549.311	114.784	1.3
4	11247.032	111.780	1.5
5	8537.424	84.850	0.5
6	8022.243	79.730	0.5
7	7779.548	77.318	3.4
8	7747.576	77.000	3.4
9	7715.605	76.682	3.4
10	4395.627	43.686	1.4
11	4087.535	40.624	1.6
12	3368.897	33.482	1.6
13	3336.198	33.157	2.3
14	2930.738	29.127	0.9
15	2611.021	25.950	1.5
16	2507.112	24.917	1.5
17	2233.899	22.202	1.6
18	1662.040	16.518	1.5

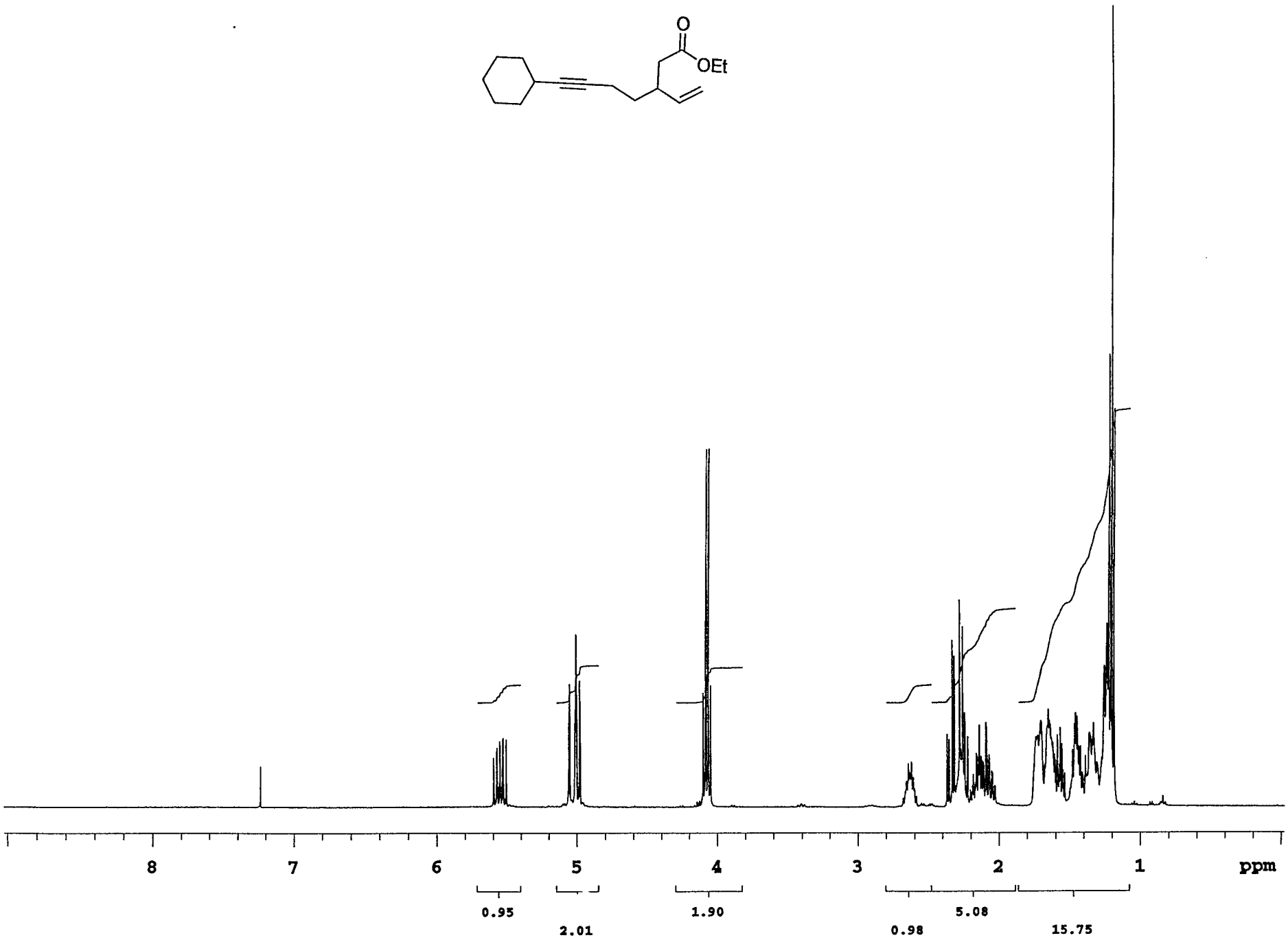




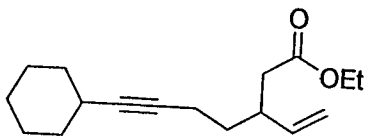


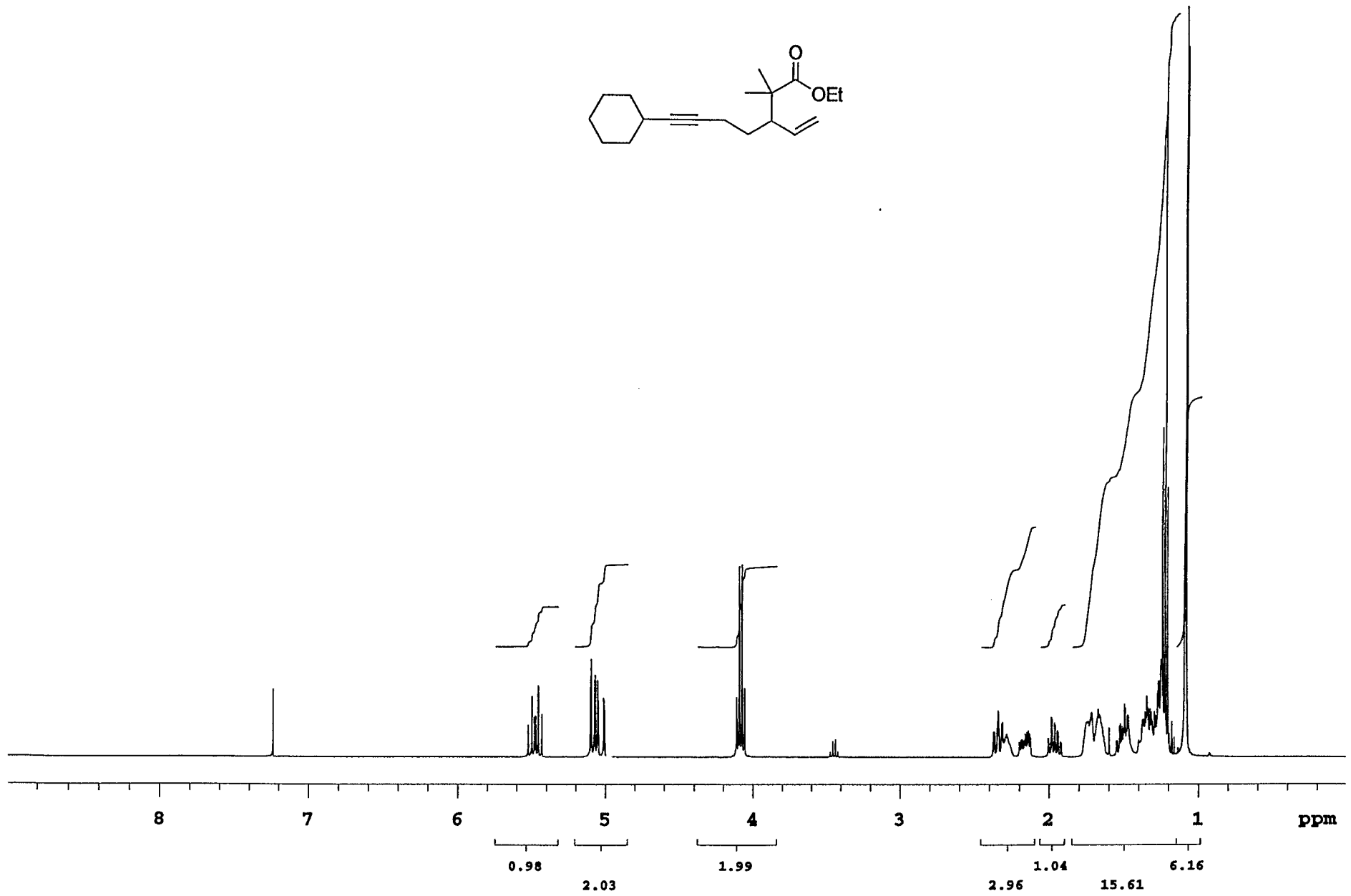
INDEX	FREQUENCY	PPM	HEIGHT
1	16748.357	166.455	0.3
2	14805.345	147.144	0.7
3	12287.568	122.121	1.0
4	8643.513	85.904	0.3
5	7868.197	78.199	0.3
6	7779.548	77.318	1.5
7	7747.576	77.000	1.6
8	7715.605	76.682	1.6
9	6051.619	60.145	0.8
10	3311.493	32.912	1.4
11	3201.772	31.821	1.0
12	2915.479	28.976	0.6
13	2602.301	25.863	1.0
14	2494.033	24.787	0.8
15	1787.747	17.768	1.0
16	1429.518	14.207	0.9



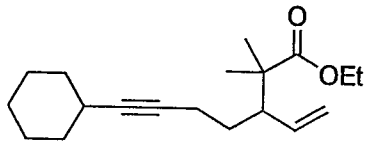


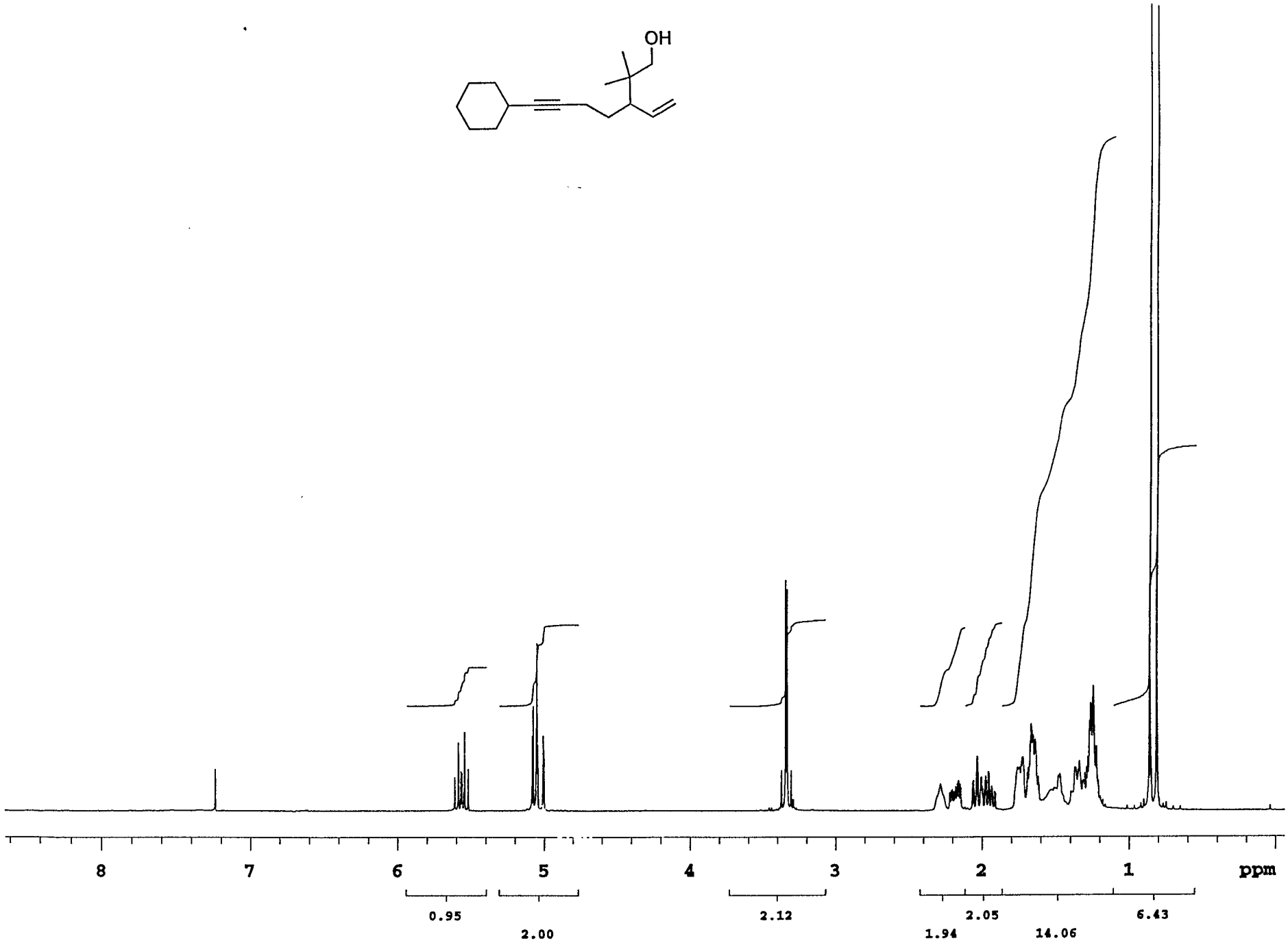
INDEX	FREQUENCY	PPM	HEIGHT
1	17325.302	172.189	0.5
2	14080.167	139.937	1.0
3	11657.579	115.860	0.9
4	8559.950	85.074	0.4
5	7964.112	79.152	0.4
6	7779.548	77.318	1.9
7	7747.576	77.000	2.0
8	7715.605	76.682	2.0
9	6055.252	60.181	0.9
10	4009.059	39.844	1.0
11	3989.440	39.649	1.1
12	3388.516	33.677	1.1
13	3325.299	33.049	1.5
14	2924.199	29.062	0.7
15	2605.208	25.892	1.1
16	2503.479	24.881	1.0
17	1655.501	16.453	1.1
18	1430.245	14.215	1.0



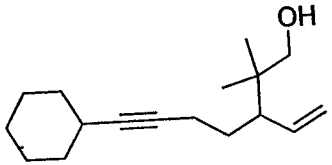


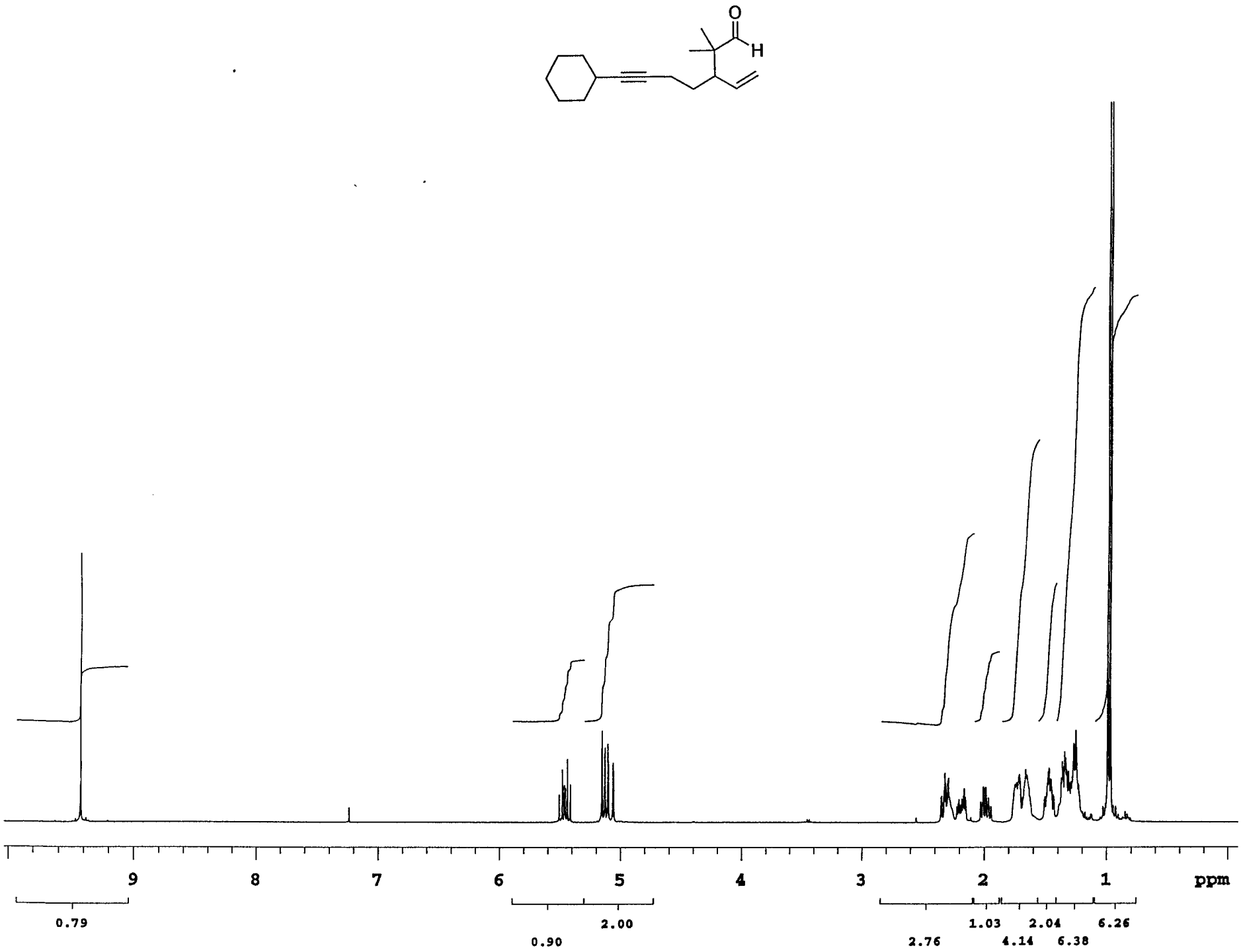
INDEX	FREQUENCY	PPM	HEIGHT
1	17852.109	177.425	1.1
2	13804.047	137.193	2.1
3	11916.259	118.431	2.0
4	8541.784	84.893	0.7
5	7997.537	79.484	0.9
6	7779.548	77.318	7.5
7	7747.576	77.000	7.7
8	7715.605	76.682	7.6
9	6063.245	60.260	2.0
10	5117.898	50.865	2.1
11	4540.953	45.131	1.6
12	3332.565	33.121	3.0
13	2927.832	29.099	1.3
14	2917.659	28.997	2.3
15	2608.114	25.921	2.1
16	2505.659	24.903	1.8
17	2347.253	23.328	2.0
18	2163.416	21.501	1.9
19	1715.811	17.053	2.3
20	1429.518	14.207	2.0



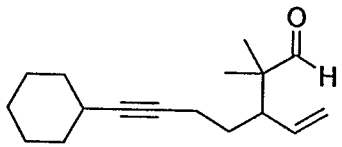


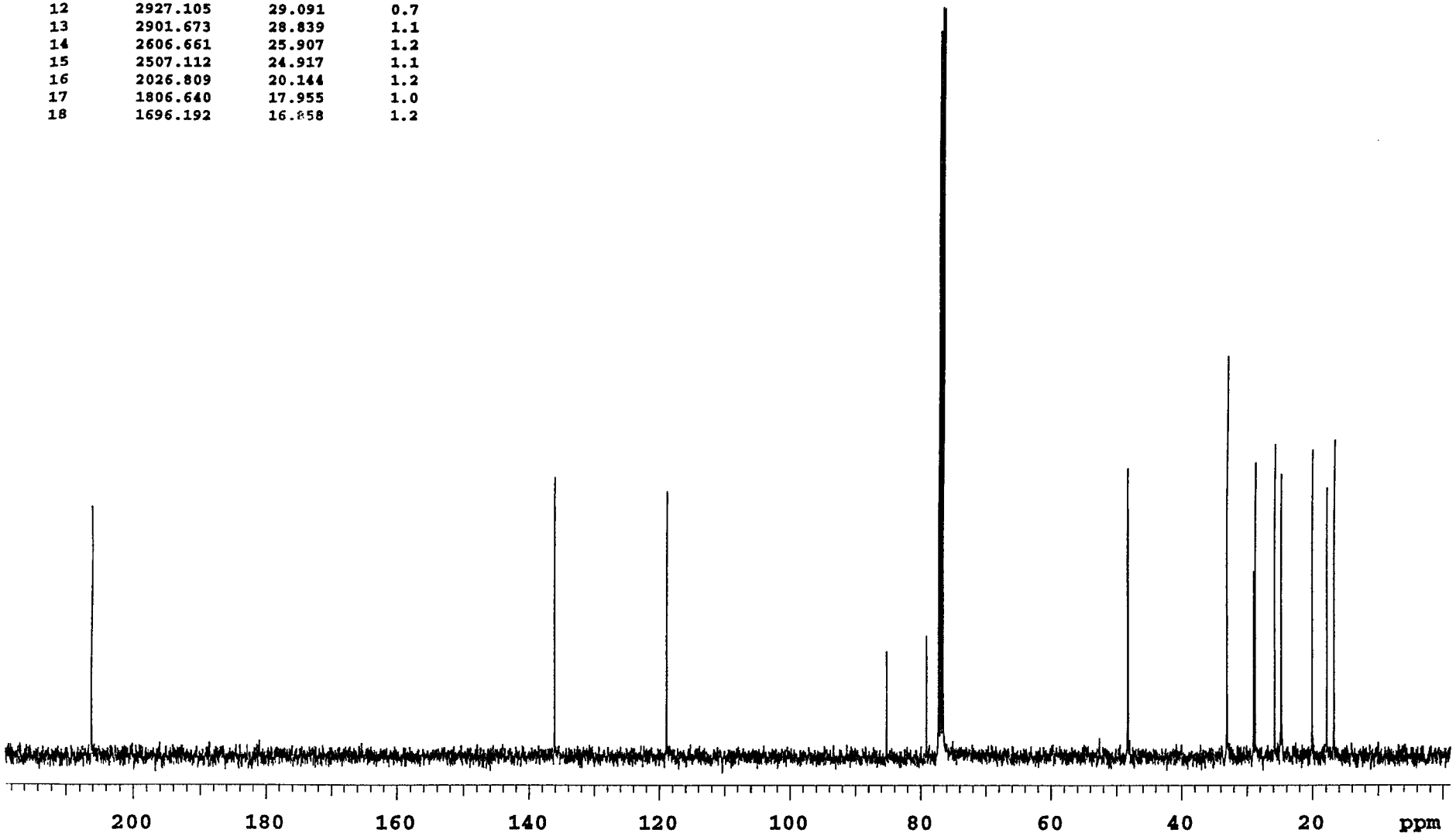
INDEX	FREQUENCY	PPM	HEIGHT
1	13981.345	138.955	0.6
2	11780.379	117.080	0.6
3	8543.964	84.915	0.2
4	8049.128	79.997	0.3
5	7779.548	77.318	2.2
6	7747.576	77.000	2.2
7	7715.605	76.682	2.2
8	7161.185	71.172	0.7
9	4964.579	49.341	0.7
10	3756.191	37.331	0.5
11	3337.652	33.172	0.9
12	2930.738	29.127	0.4
13	2823.924	28.066	0.7
14	2605.934	25.899	0.7
15	2510.745	24.953	0.6
16	2229.539	22.158	0.6
17	2137.257	21.241	0.6
18	1719.444	17.089	0.7

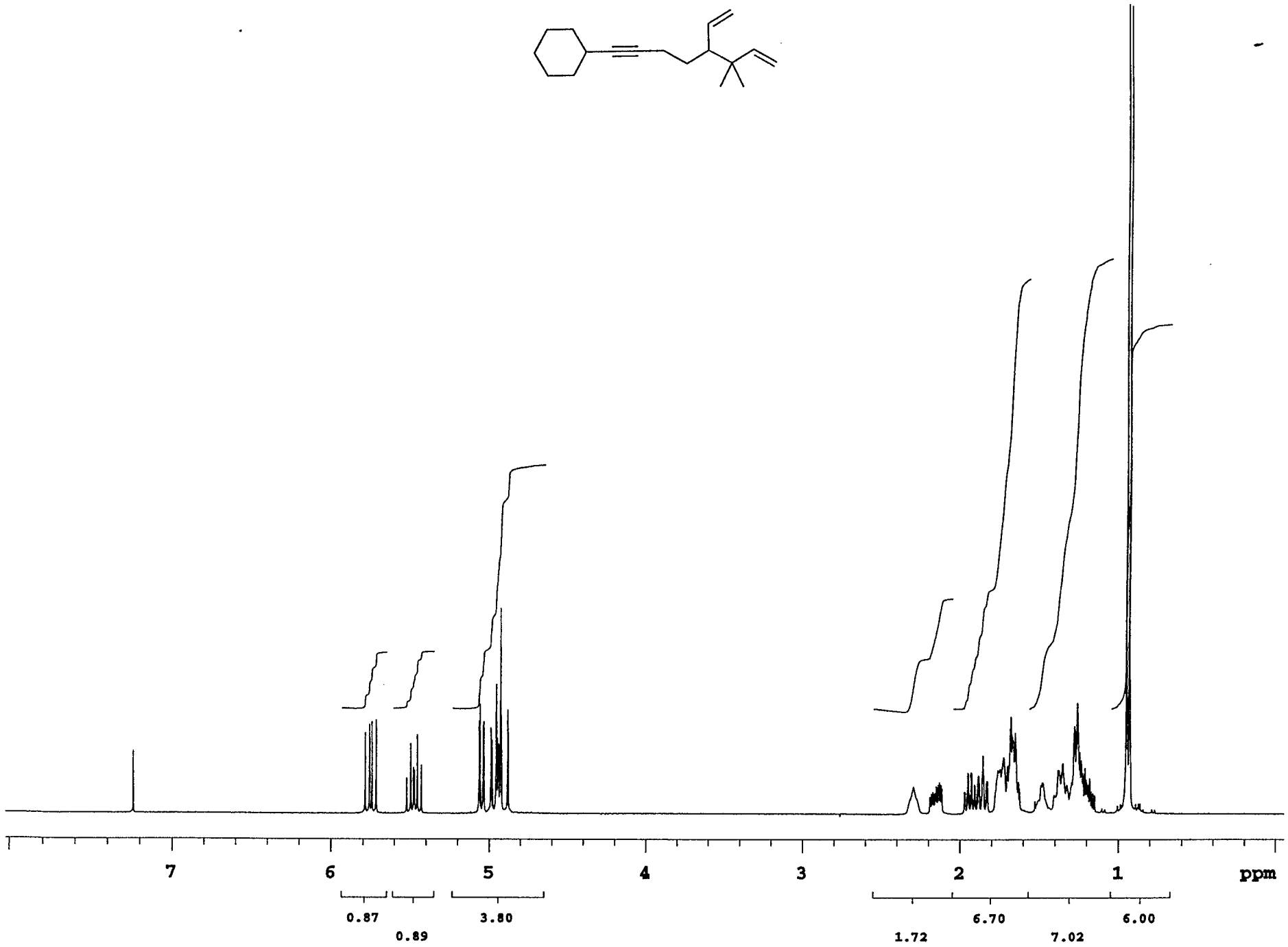




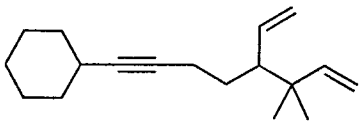
INDEX	FREQUENCY	PPM	HEIGHT
1	20747.008	206.196	1.0
2	13704.499	136.203	1.1
3	11969.303	118.958	1.0
4	8579.569	85.269	0.4
5	7967.019	79.181	0.5
6	7779.548	77.318	2.8
7	7747.576	77.000	2.9
8	7715.605	76.682	2.9
9	4868.664	48.388	1.1
10	4858.491	48.287	1.0
11	3334.019	33.135	1.5
12	2927.105	29.091	0.7
13	2901.673	28.839	1.1
14	2606.661	25.907	1.2
15	2507.112	24.917	1.1
16	2026.809	20.144	1.2
17	1806.640	17.955	1.0
18	1696.192	16.858	1.2

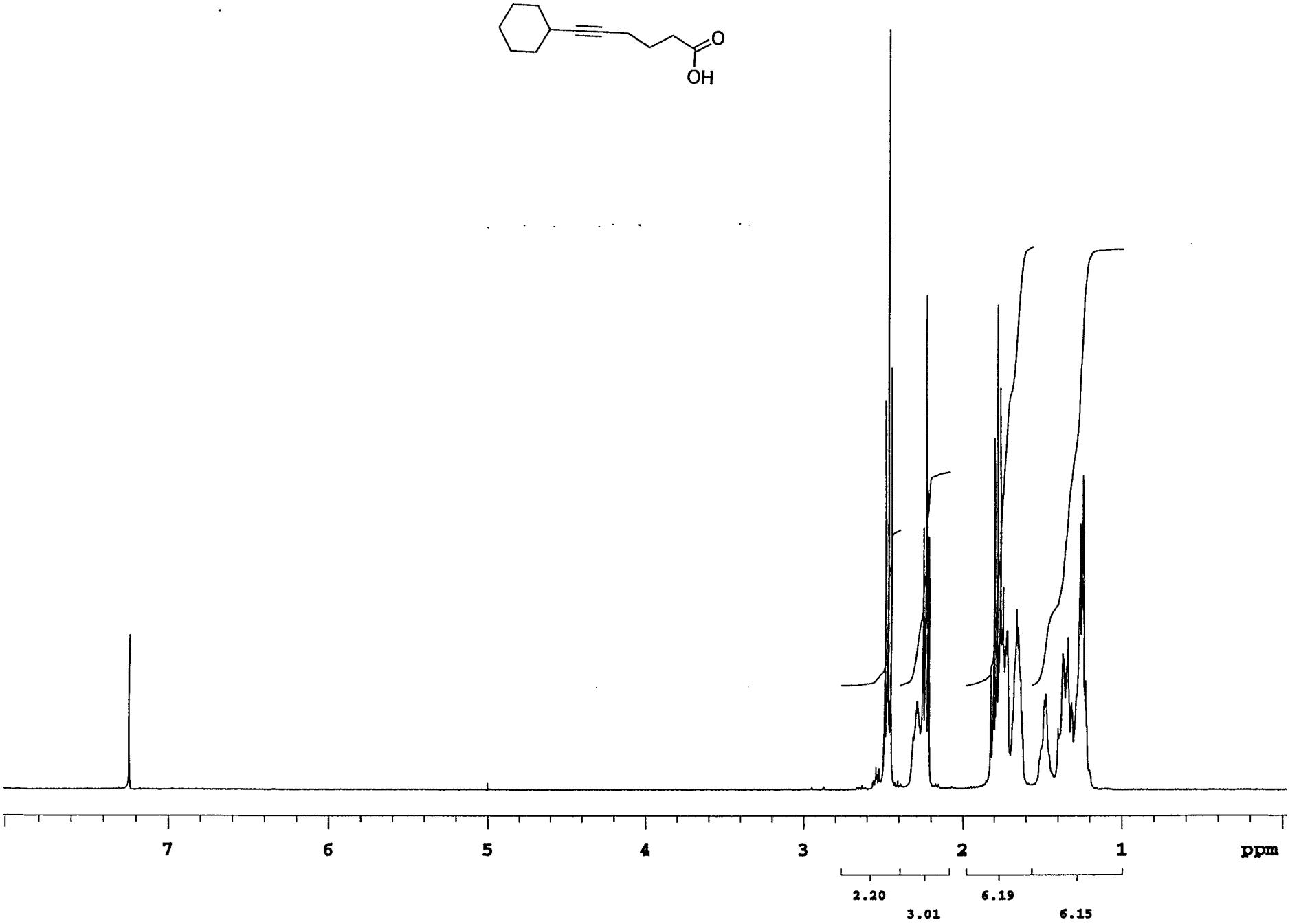




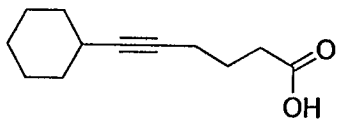


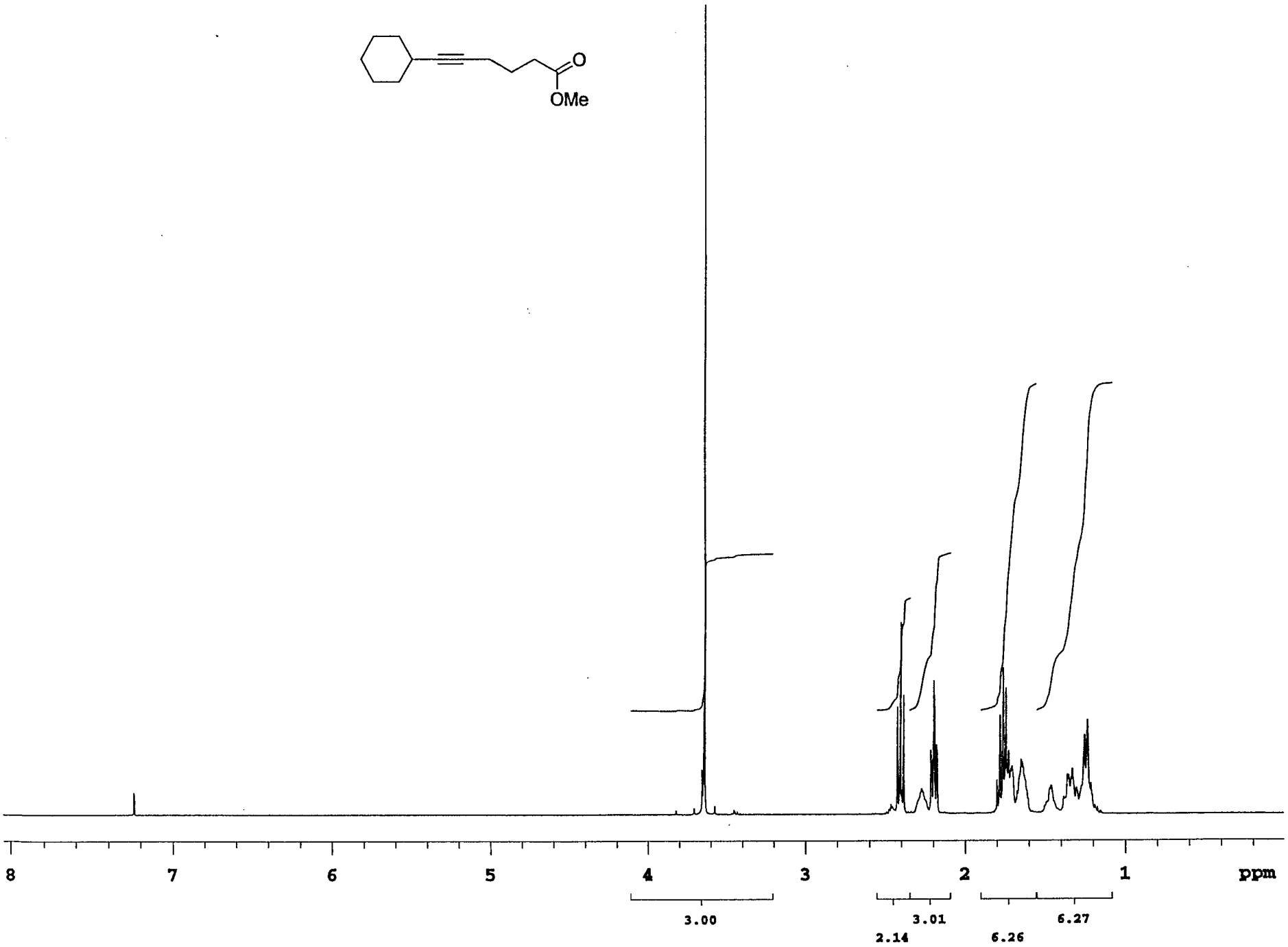
INDEX	FREQUENCY	PPM	HEIGHT
1	14811.158	147.202	0.7
2	13947.920	138.623	0.7
3	11783.286	117.109	0.7
4	11196.894	111.281	0.7
5	8521.439	84.691	0.3
6	8049.855	80.004	0.3
7	7779.548	77.318	3.1
8	7747.576	77.000	3.1
9	7715.605	76.682	3.1
10	5360.593	53.277	0.8
11	3905.151	38.812	0.6
12	3340.558	33.200	1.1
13	2932.192	29.142	0.5
14	2890.047	28.723	0.8
15	2656.072	26.398	0.7
16	2611.747	25.957	0.8
17	2510.019	24.946	0.7
18	2334.174	23.198	0.7
19	1728.164	17.176	0.8



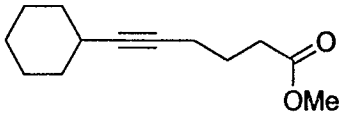


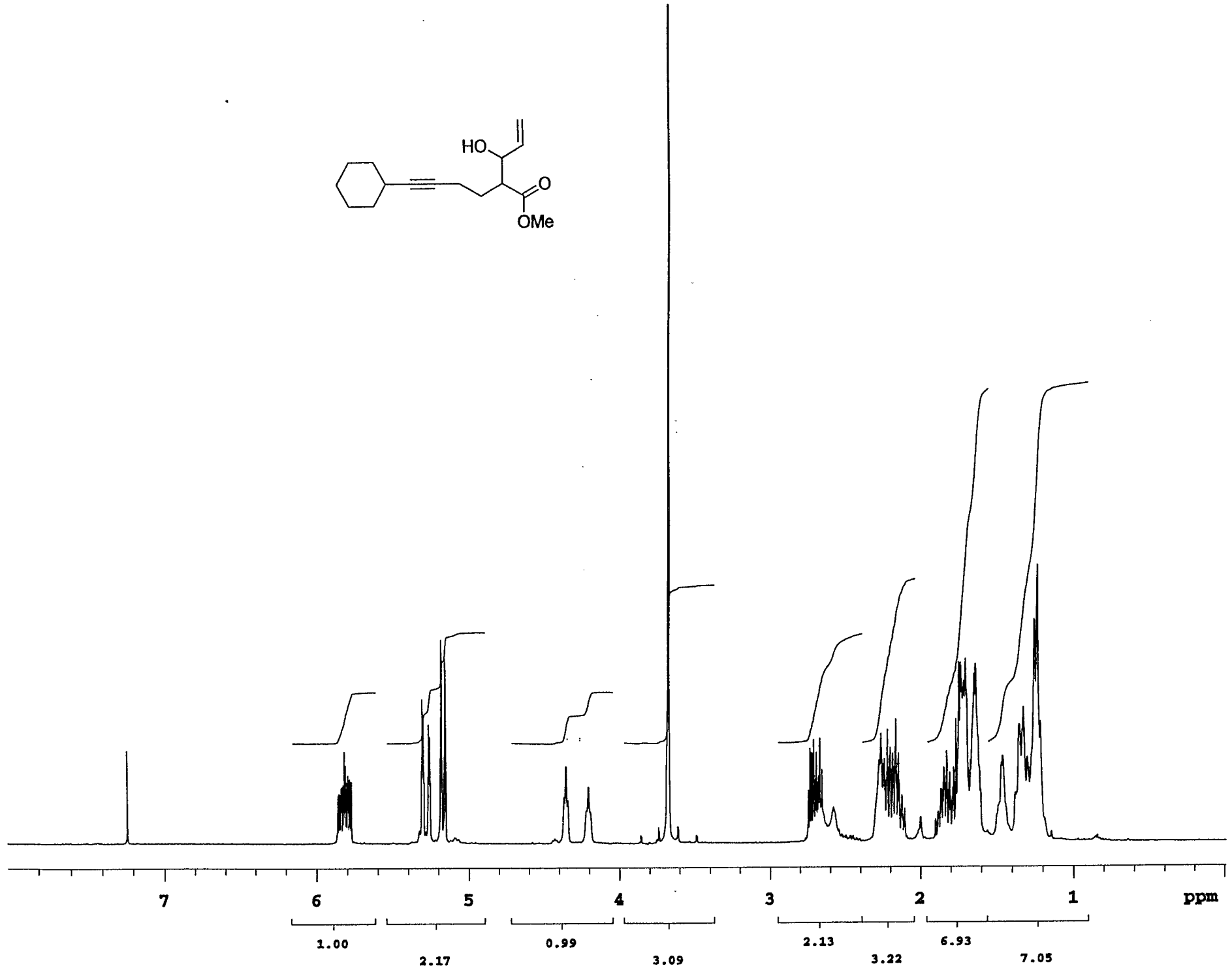
INDEX	FREQUENCY	PPM	HEIGHT
1	18097.711	179.866	0.2
2	8642.059	85.890	0.2
3	7882.003	78.336	0.3
4	7779.548	77.318	2.3
5	7747.576	77.000	2.3
6	7715.605	76.682	2.3
7	3324.572	33.042	1.0
8	3297.687	32.774	0.5
9	2927.832	29.099	0.4
10	2605.208	25.892	0.7
11	2509.292	24.939	0.6
12	2409.017	23.942	0.6
13	1824.806	18.136	0.6



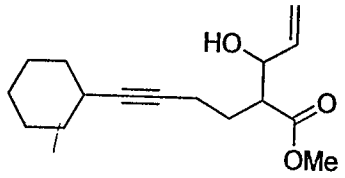


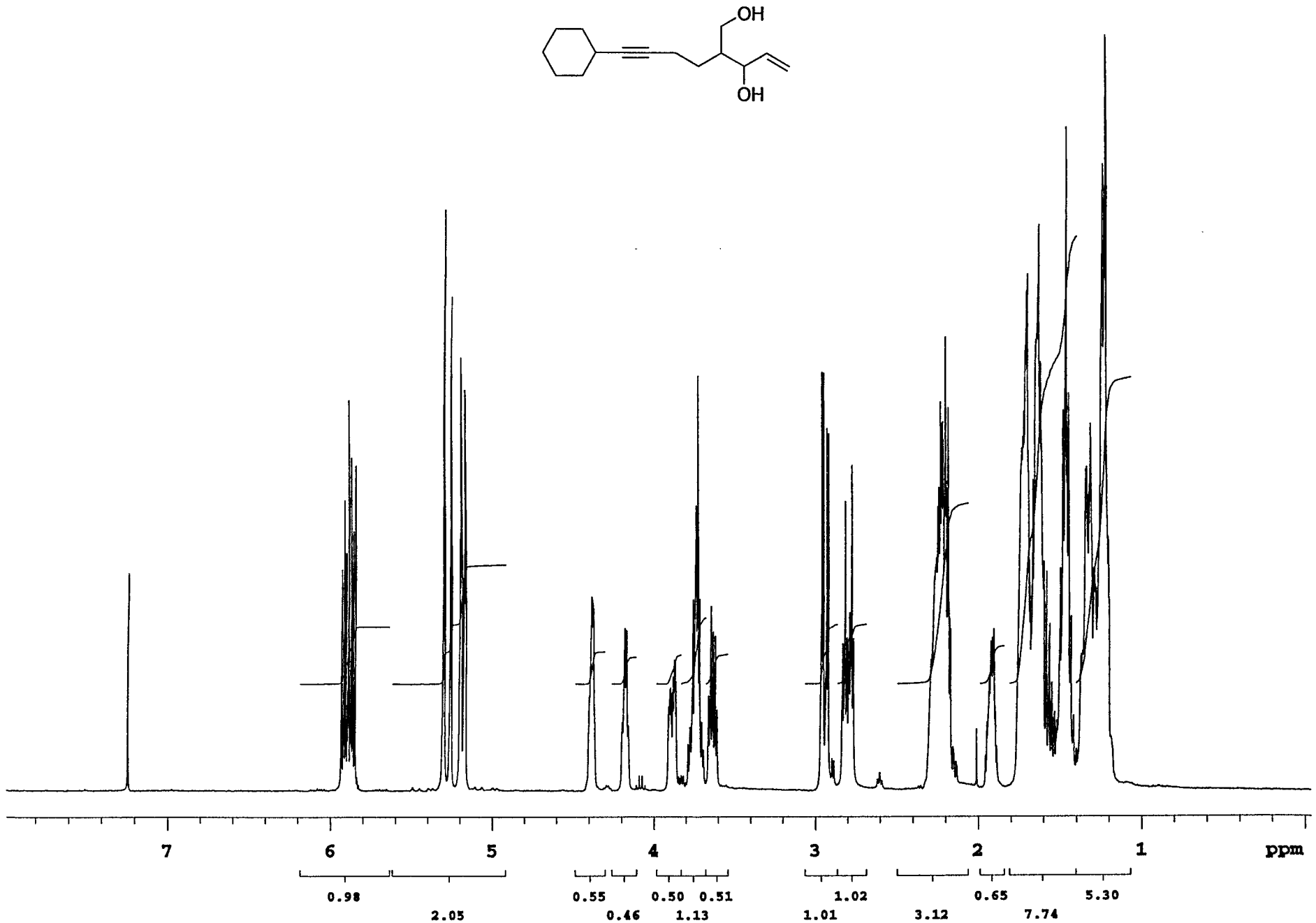
INDEX	FREQUENCY	PPM	HEIGHT
1	17485.887	173.785	2.8
2	8616.627	85.637	1.7
3	7901.622	78.531	2.4
4	7779.548	77.318	8.2
5	7747.576	77.000	8.2
6	7715.605	76.682	8.0
7	5179.662	51.479	4.1
8	3326.026	33.056	8.4
9	3302.047	32.818	6.4
10	2926.379	29.084	2.9
11	2605.208	25.892	5.3
12	2505.659	24.903	3.3
13	2443.169	24.282	7.6
14	1832.072	18.208	7.9



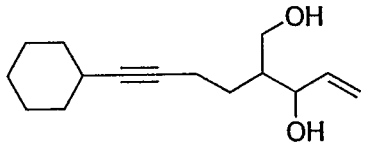


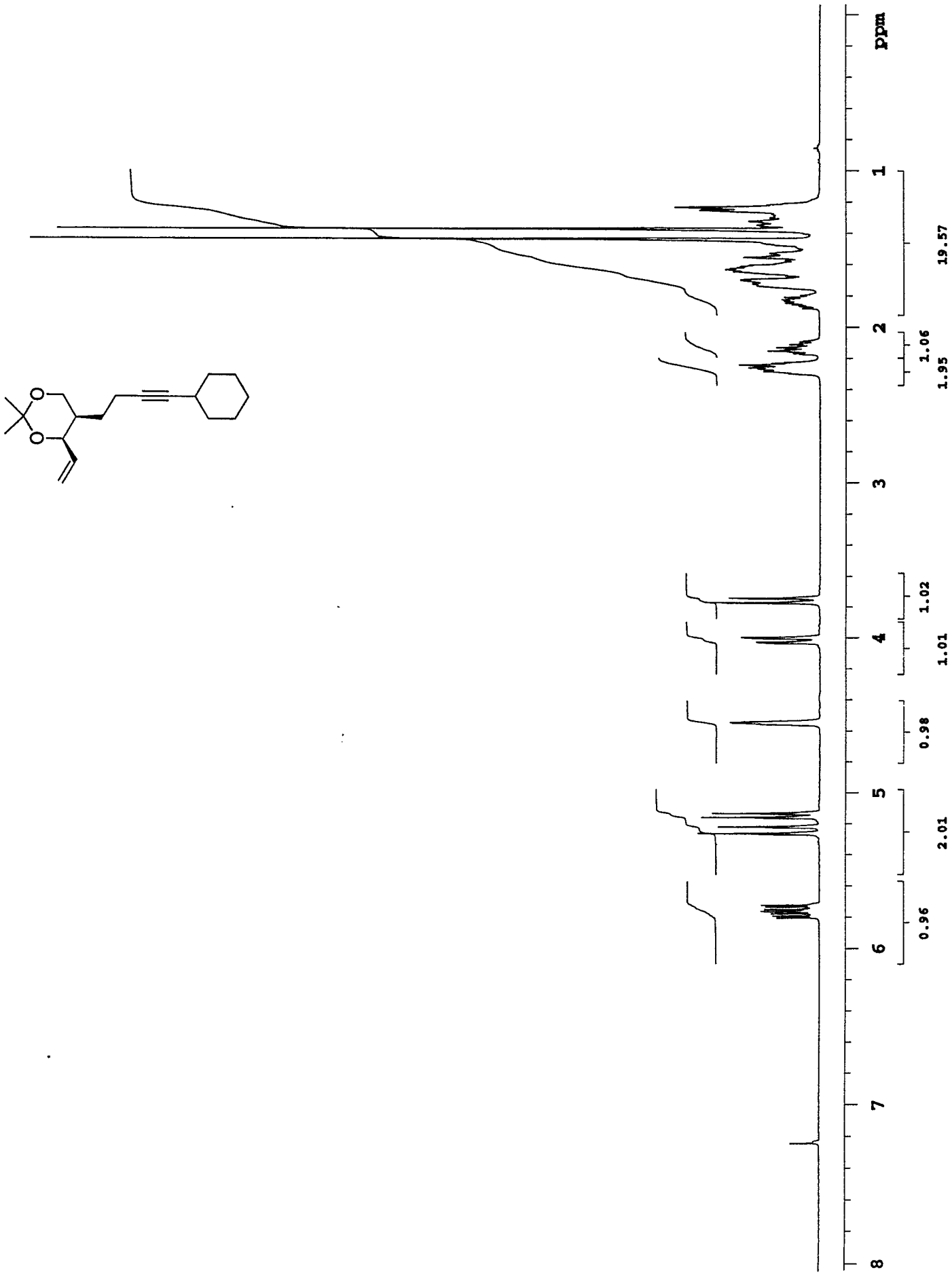
INDEX	FREQUENCY	PPM	HEIGHT
1	17616.681	175.085	0.7
2	17573.810	174.659	0.7
3	13926.121	138.406	1.2
4	13822.939	137.381	1.2
5	11724.429	116.524	1.2
6	11720.069	116.481	1.3
7	8627.527	85.745	0.4
8	8617.354	85.644	0.5
9	7903.802	78.553	0.5
10	7876.917	78.285	0.5
11	7779.548	77.318	6.8
12	7747.576	77.000	6.9
13	7715.605	76.682	6.7
14	7353.742	73.086	1.3
15	7339.936	72.949	1.5
16	5209.454	51.775	1.2
17	5202.187	51.702	1.0
18	5004.544	49.738	1.3
19	4991.464	49.608	1.4
20	3321.666	33.013	2.5
21	2924.925	29.070	1.2
22	2866.795	28.492	1.3
23	2660.432	26.441	1.3
24	2603.028	25.870	2.7
25	2504.206	24.888	1.9
26	1719.444	17.089	1.3
27	1691.106	16.807	1.2



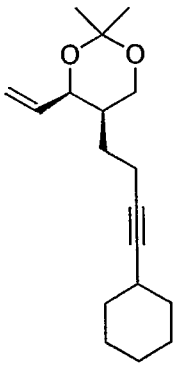


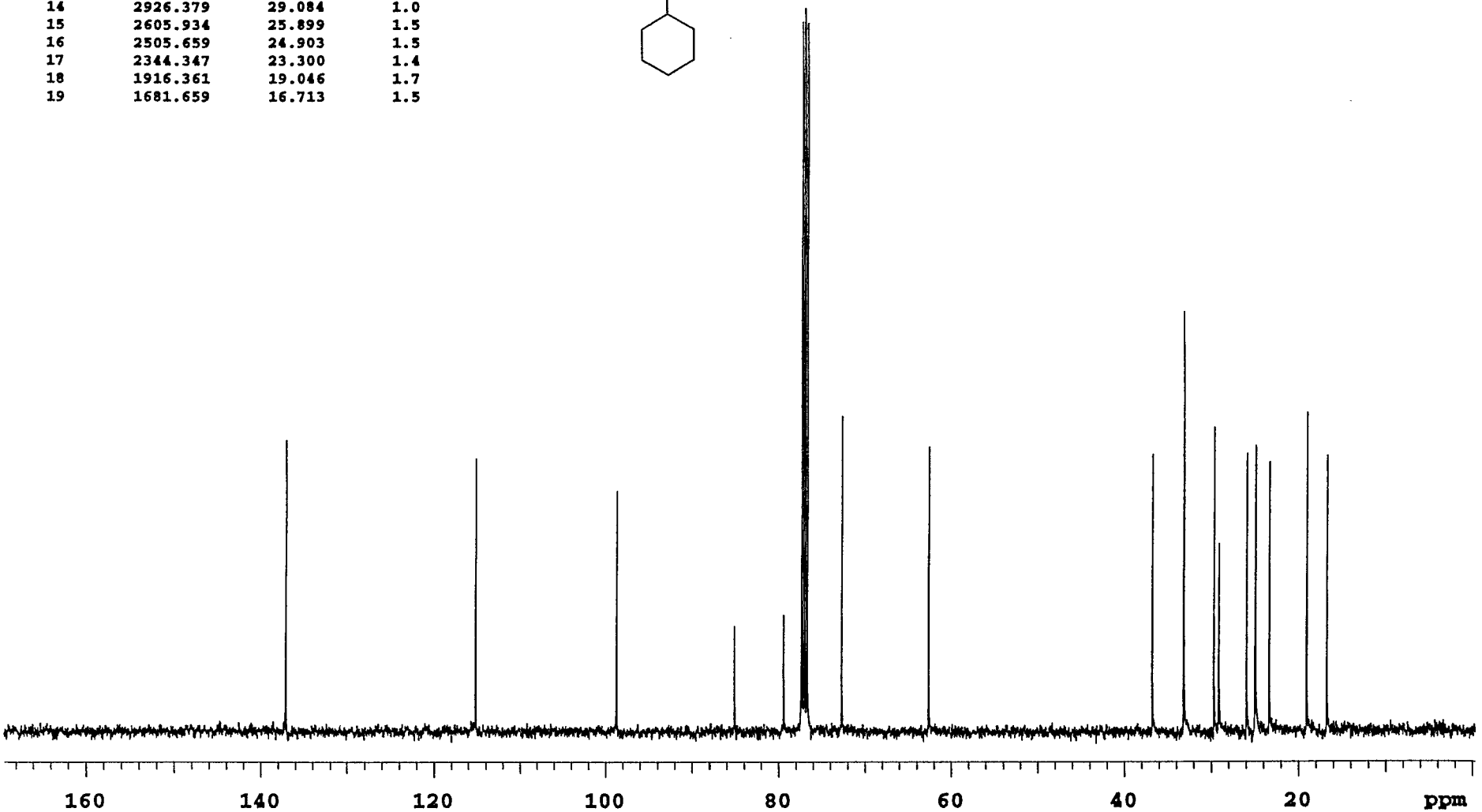
INDEX	FREQUENCY	PPM	HEIGHT
1	14072.901	139.865	0.8
2	13907.229	138.218	0.9
3	11649.586	115.780	0.9
4	11640.866	115.694	1.0
5	8589.742	85.370	0.5
6	7982.278	79.333	0.4
7	7977.918	79.289	0.4
8	7779.548	77.318	4.1
9	7747.576	77.000	4.3
10	7715.605	76.682	4.1
11	7677.820	76.307	0.9
12	7618.236	75.715	1.1
13	6438.914	63.994	1.0
14	6360.437	63.214	0.9
15	4386.181	43.592	0.9
16	4373.828	43.470	0.8
17	3326.752	33.063	2.8
18	2927.105	29.091	1.1
19	2749.807	27.329	0.9
20	2600.848	25.849	2.1
21	2512.925	24.975	1.5
22	2507.839	24.924	1.6
23	1693.285	16.829	1.0
24	1669.307	16.591	0.9

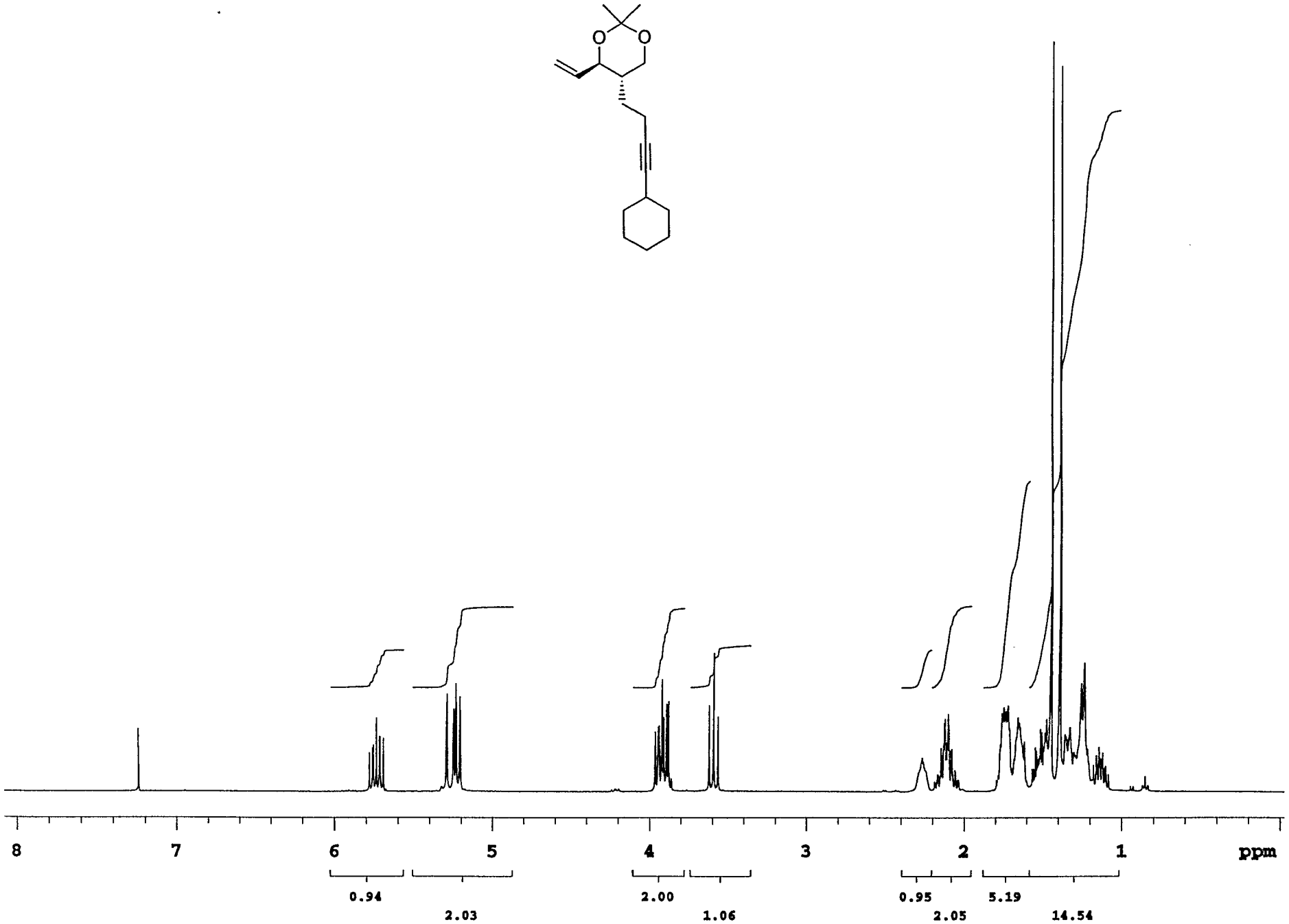



ppm
1
2
3
4
5
6
7
8
19.57
1.06
1.95
1.02
1.01
0.98
2.01
0.96

INDEX	FREQUENCY	PPM	HEIGHT
1	13794.601	137.099	1.5
2	11584.189	115.131	1.4
3	9931.103	98.701	1.3
4	8560.677	85.081	0.6
5	7986.638	79.376	0.6
6	7779.548	77.318	3.8
7	7747.576	77.000	3.8
8	7715.605	76.682	3.8
9	7311.598	72.667	1.7
10	6299.400	62.607	1.5
11	3699.514	36.768	1.5
12	3331.839	33.114	2.2
13	2984.509	29.662	1.6
14	2926.379	29.084	1.0
15	2605.934	25.899	1.5
16	2505.659	24.903	1.5
17	2344.347	23.300	1.4
18	1916.361	19.046	1.7
19	1681.659	16.713	1.5







INDEX	FREQUENCY	PPM	HEIGHT
1	13782.248	136.976	1.4
2	11932.972	118.597	1.2
3	9866.433	98.058	1.3
4	8583.929	85.312	0.5
5	7938.680	78.899	0.6
6	7779.548	77.318	4.4
7	7747.576	77.000	4.5
8	7715.605	76.682	4.5
9	7650.208	76.032	1.4
10	6432.374	63.929	1.5
11	3811.415	37.880	1.5
12	3323.846	33.034	2.2
13	2980.876	29.626	1.6
14	2927.832	29.099	1.0
15	2770.153	27.531	1.5
16	2602.301	25.863	1.6
17	2510.019	24.946	1.5
18	1933.800	19.219	1.6
19	1630.795	16.208	1.4