

Terms & Conditions

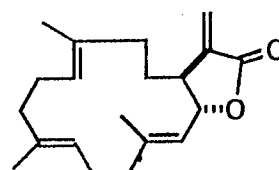
Electronic Supporting Information files are available without a subscription to ACS Web Editions. The American Chemical Society holds a copyright ownership interest in any copyrightable Supporting Information. Files available from the ACS website may be downloaded for personal use only. Users are not otherwise permitted to reproduce, republish, redistribute, or sell any Supporting Information from the ACS website, either in whole or in part, in either machine-readable form or any other form without permission from the American Chemical Society. For permission to reproduce, republish and redistribute this material, requesters must process their own requests via the RightsLink permission system. Information about how to use the RightsLink permission system can be found at <http://pubs.acs.org/page/copyright/permissions.html>



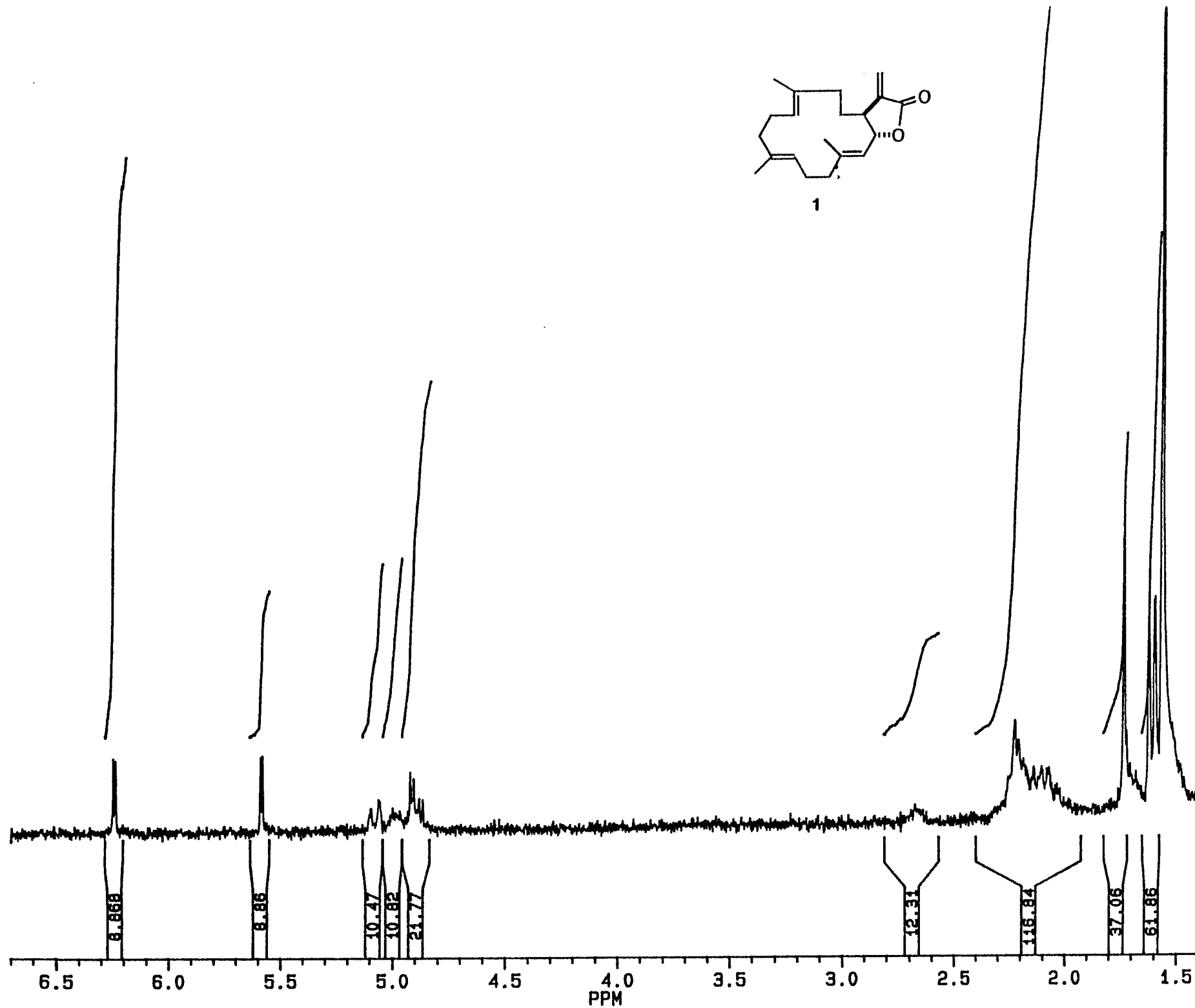
ACS Publications

MOST TRUSTED. MOST CITED. MOST READ.

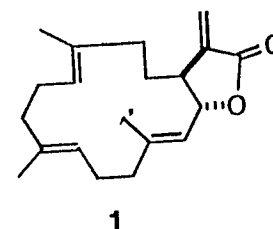
Copyright © 1997 American Chemical Society



1



	[Hz]	[Hz]	[PPM]	
1	13144.7	14214.199	141.2763	0.86
2	13211.2	14159.056	140.7282	0.90
3	14075.7	13442.083	133.6022	0.94
4	14355.9	13209.751	131.2930	1.15
5	15008.6	12668.506	125.9135	-3.12
6	15081.9	12607.713	125.3093	-3.41
7	15311.8	12417.010	123.4138	-3.42
8	15546.9	12222.110	121.4767	2.97
9	20680.7	7964.708	79.1620	-3.74
10	20904.0	7779.556	77.3218	54.12
11	20942.5	7747.570	77.0038	54.29
12	20981.0	7715.692	76.6870	55.18
13	25072.8	4322.435	42.9611	-3.58
14	25562.2	3916.594	38.9274	3.27
15	25630.0	3860.306	38.3680	3.11
16	25917.0	3622.317	36.0026	3.45
17	26385.8	3233.563	32.1387	3.24
18	27367.9	2419.118	24.0438	3.65
19	27392.1	2399.029	23.8442	3.40
20	27574.9	2247.443	22.3376	1.67



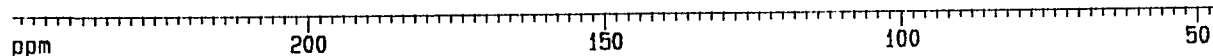
Current Data Parameters
NAME cem
EXPNO 1
PROCNO 1

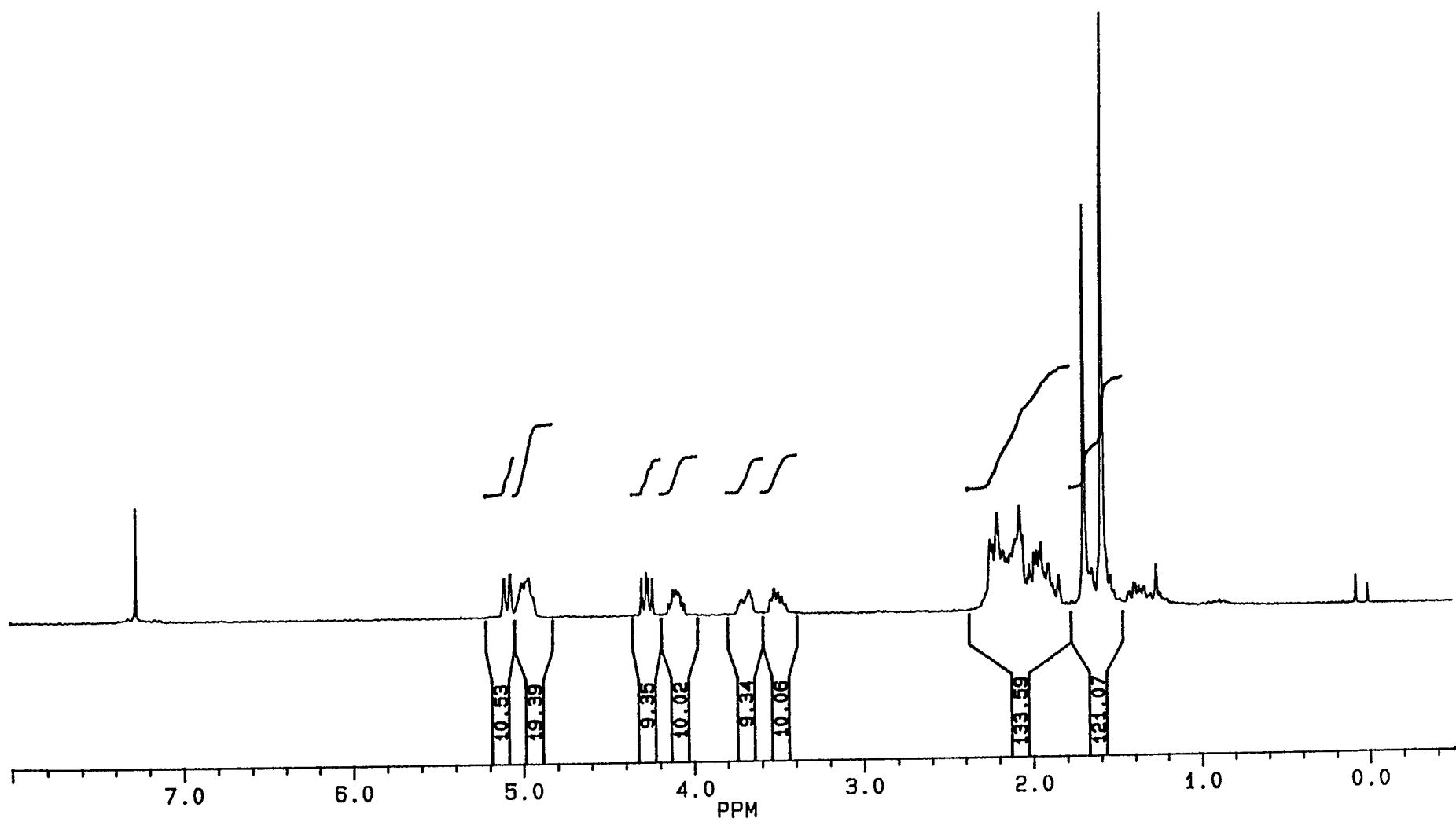
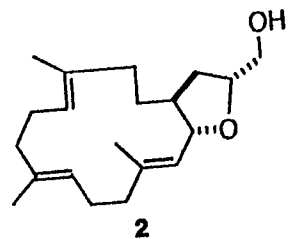
F2 - Acquisition Parameters
Date_ 961029
Time 15.14
INSTRUM spect
PROBHD 5 mm GNP 1H
PULPROG jvert
TD 65536
SOLVENT CDCl3
NS 14638
DS 0
SWH 27173.912 Hz
FIDRES 0.414641 Hz
AQ 1.2059124 sec
RG 2048
DM 18.400 usec
DE 4.50 usec
TE 300.0 K
D11 0.03000000 sec
PL12 18.00 dB
D1 3.00000000 sec
CPDPRG2 waltz16
PCPD2 95.00 usec
SF02 400.1320007 MHz
NUC2 1H
PL2 120.00 dB
D13 0.00000300 sec
P1 10.50 usec
D20 0.00700000 sec
P2 21.00 usec
DE 4.50 usec
SF01 100.6242995 MHz
NUC1 13C
PL1 0.00 dB

F2 - Processing parameters
SI 32768
SF 100.6127716 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

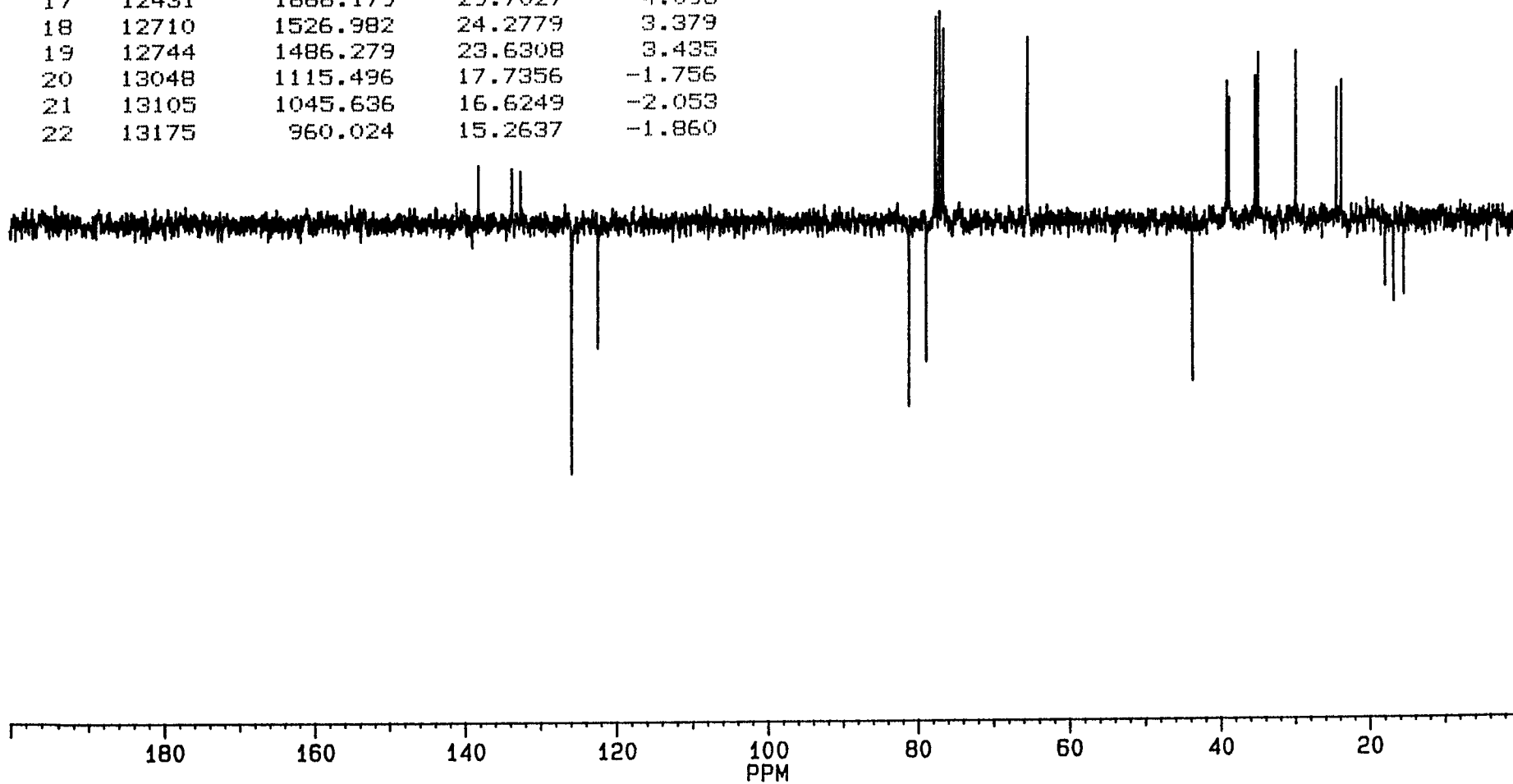
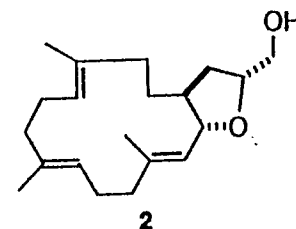
1D NMR plot parameters
CX 20.00 cm
F1P 249.619 ppm
F1 25114.84 Hz
F2P 1.000 ppm
F2 100.61 Hz
PPMCM 12.43094 ppm/cm
HZCM 1250.71130 Hz/cm

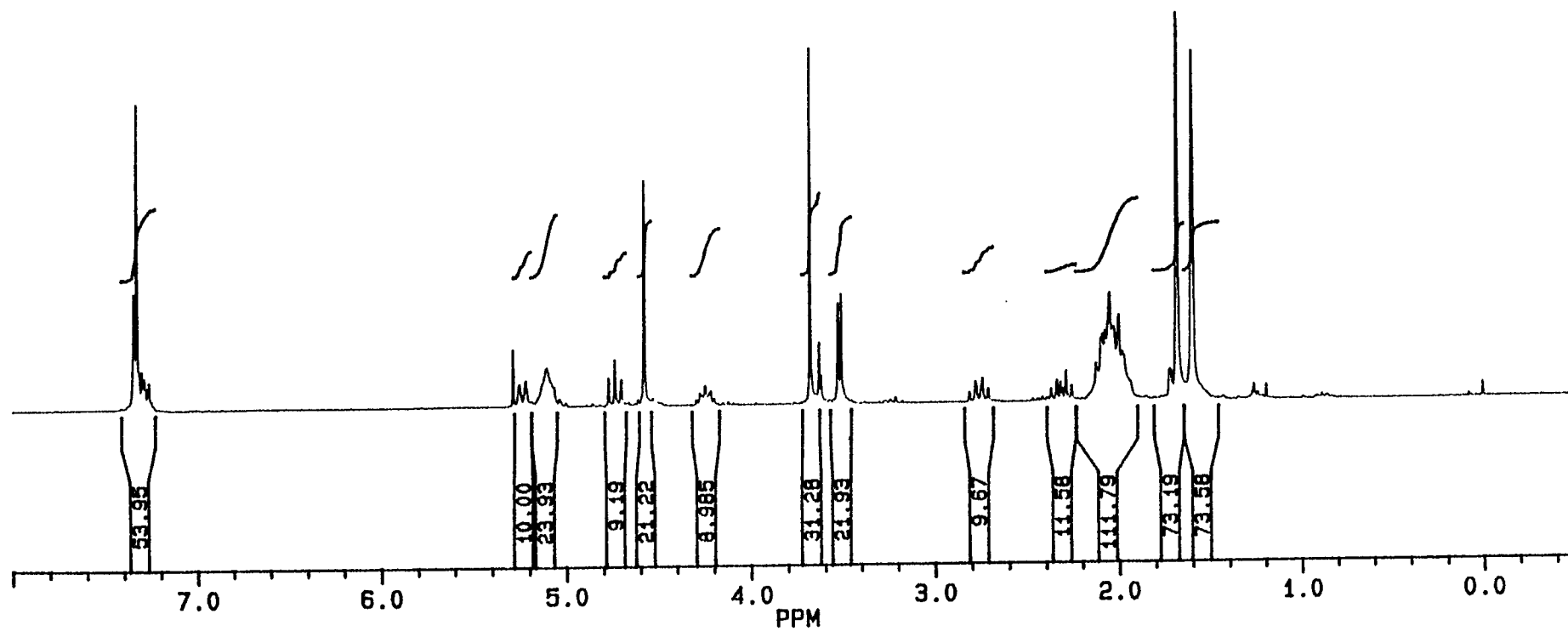
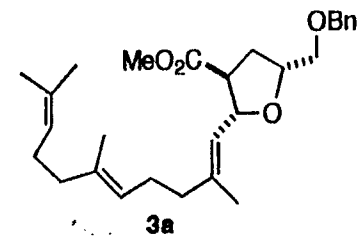
21	28291.9	1652.853	16.4279	-1.45
22	28387.2	1573.870	15.6428	-1.22
23	28438.3	1531.502	15.2218	-1.31
24	28578.8	1414.961	14.0634	-1.93

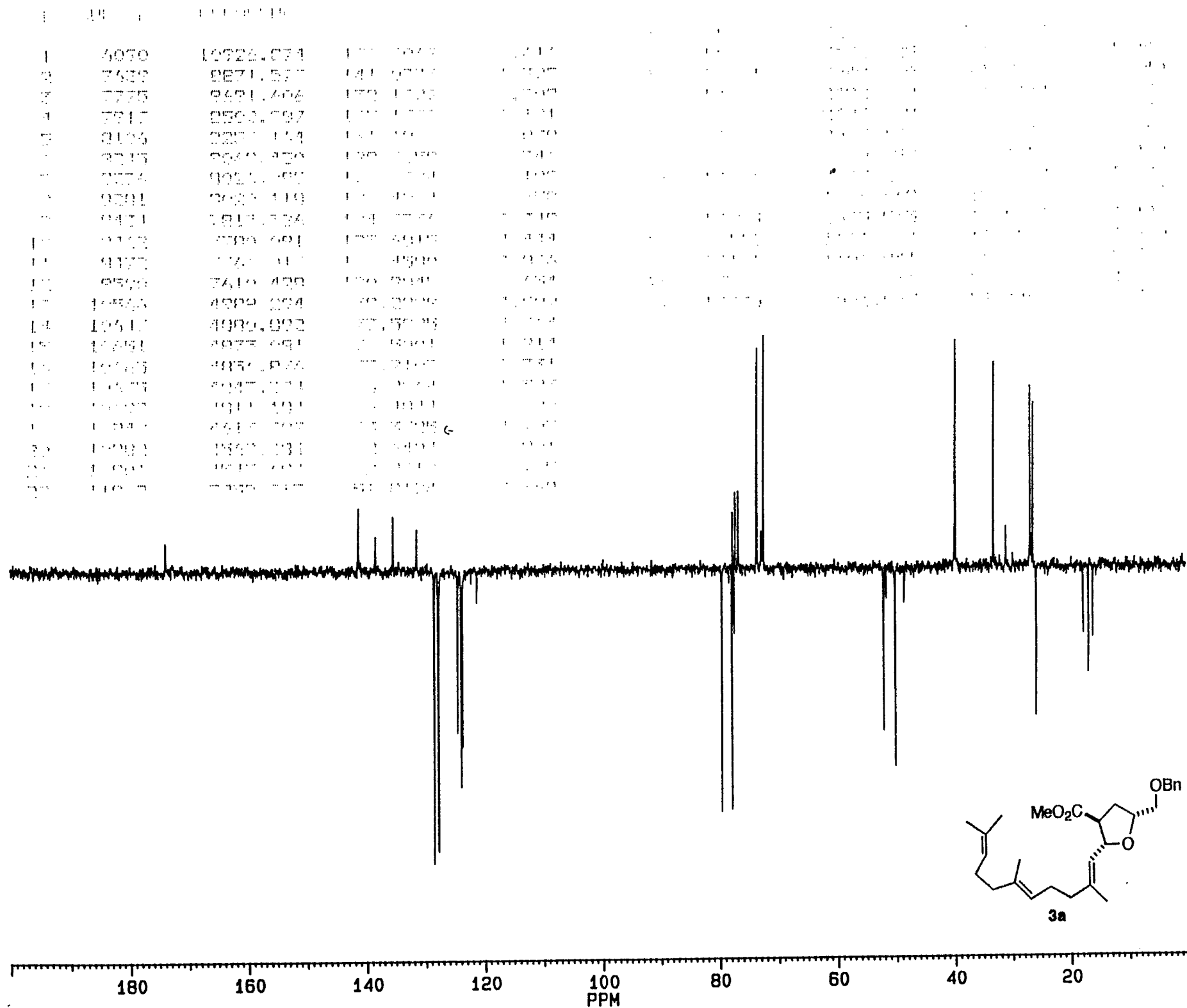


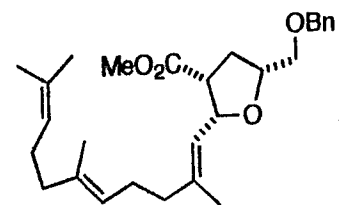


#	CURSOR	FREQUENCY	PPM	INTENSITY
1	6848	8683.222	138.0569	1.395
2	7076	8405.526	133.6418	1.370
3	7134	8334.018	132.5048	1.263
4	7483	7908.277	125.7359	-6.010
5	7661	7690.718	122.2768	-3.056
6	9788	5094.335	80.9962	-4.450
7	9906	4949.875	78.6994	-3.595
8	9968	4874.563	77.5020	4.980
9	9994	4842.702	76.9954	5.169
10	10021	4810.606	76.4851	4.890
11	10597	4106.673	65.2931	4.514
12	11719	2737.520	43.5246	-3.937
13	11954	2450.193	38.9563	3.404
14	11971	2429.215	38.6227	3.098
15	12151	2209.983	35.1371	3.501
16	12170	2186.537	34.7643	4.118
17	12431	1868.179	29.7027	4.098
18	12710	1526.982	24.2779	3.379
19	12744	1486.279	23.6308	3.435
20	13048	1115.496	17.7356	-1.756
21	13105	1045.636	16.6249	-2.053
22	13175	960.024	15.2637	-1.860

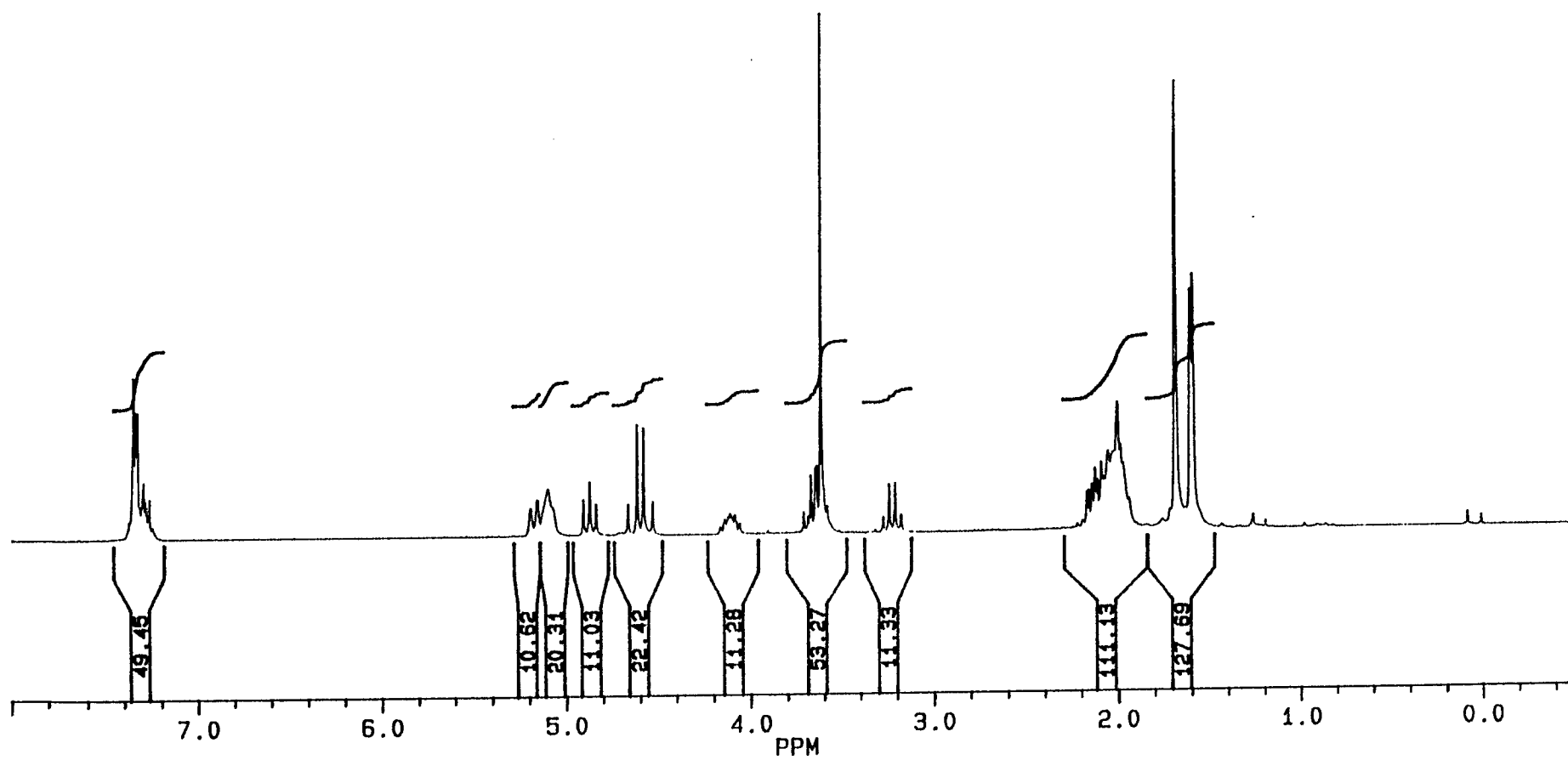


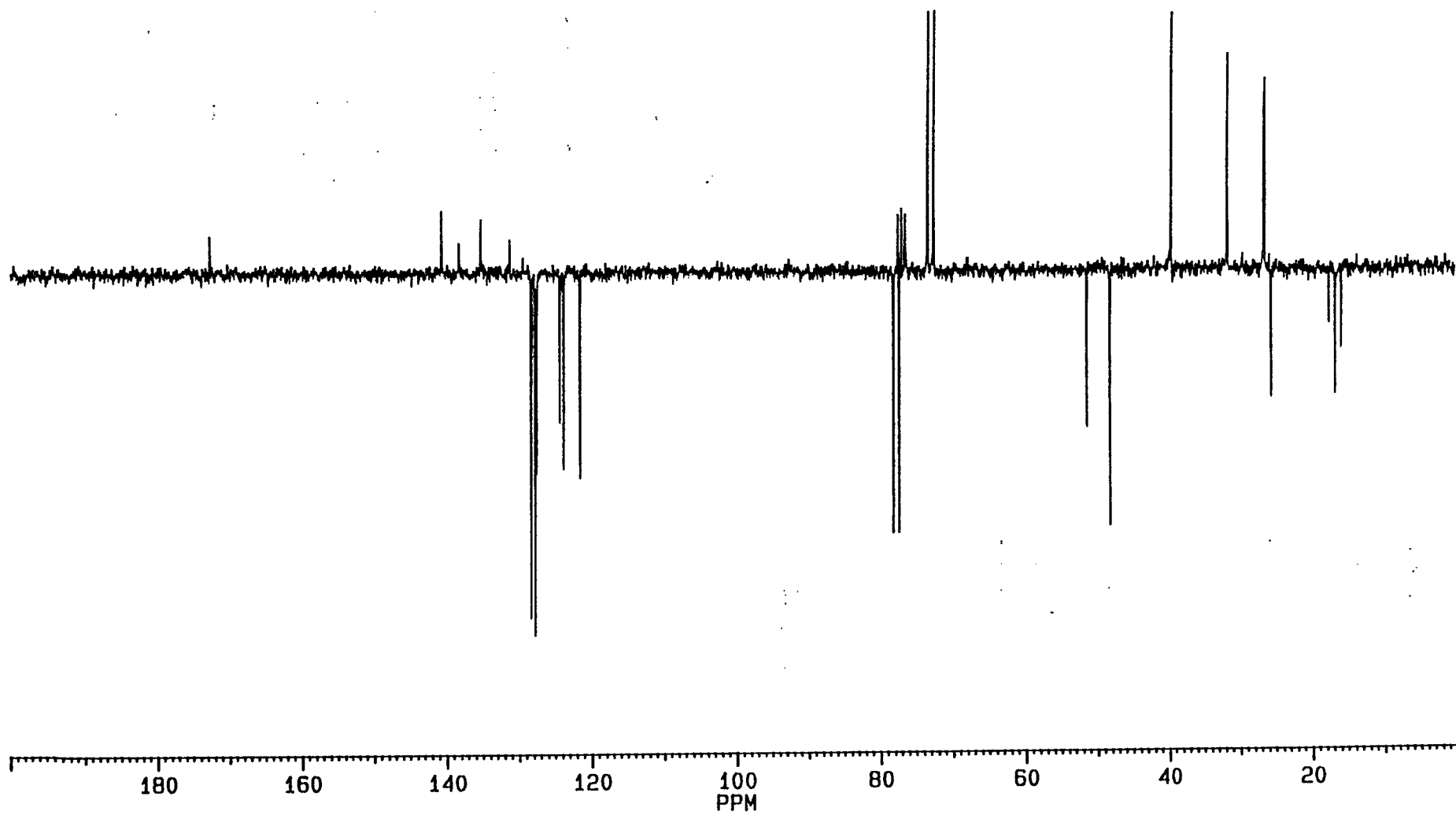
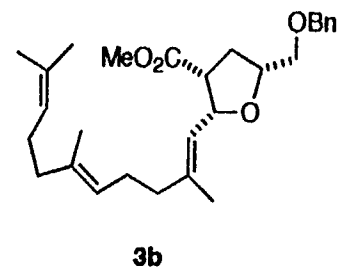


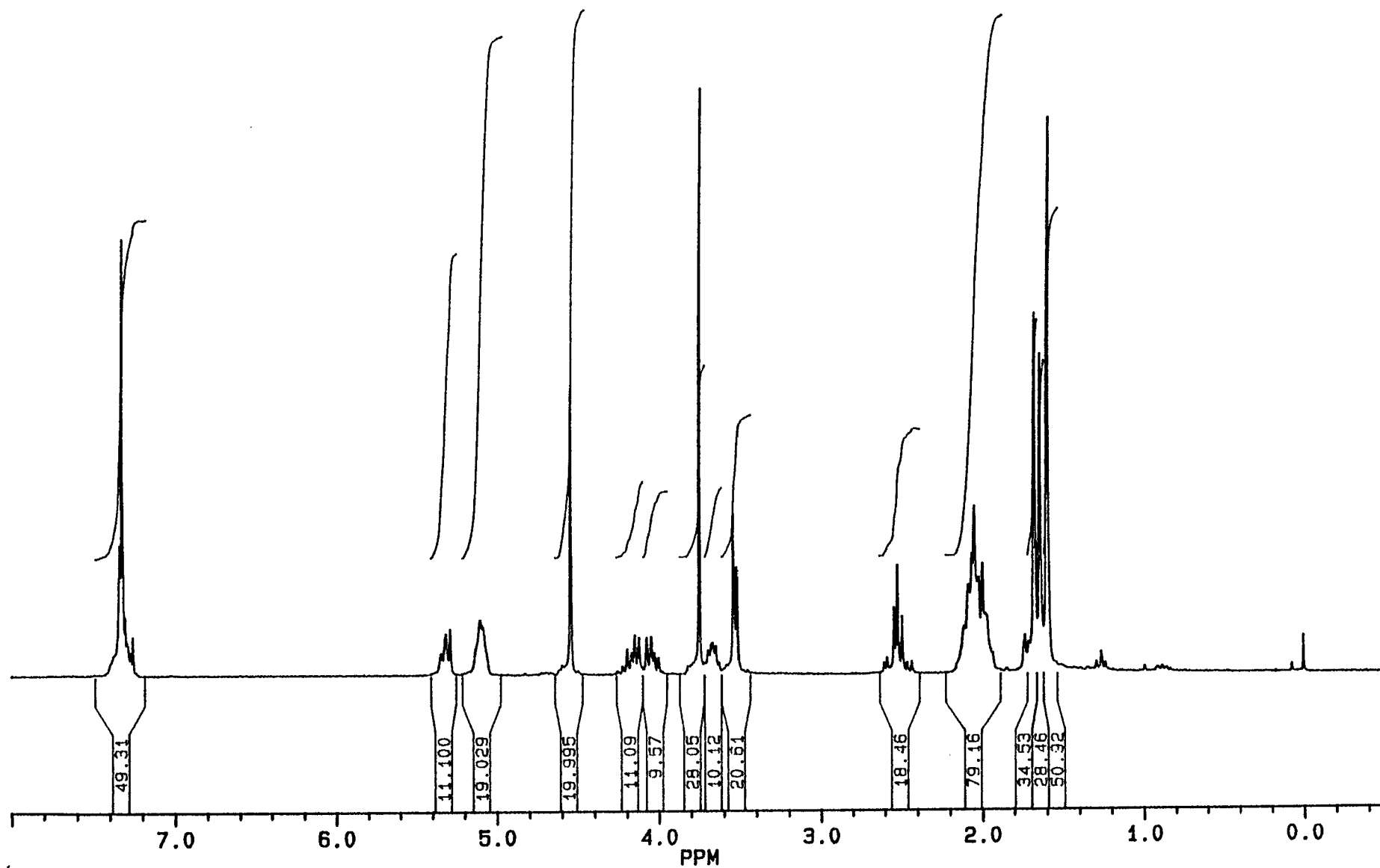
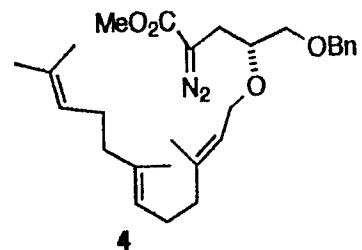




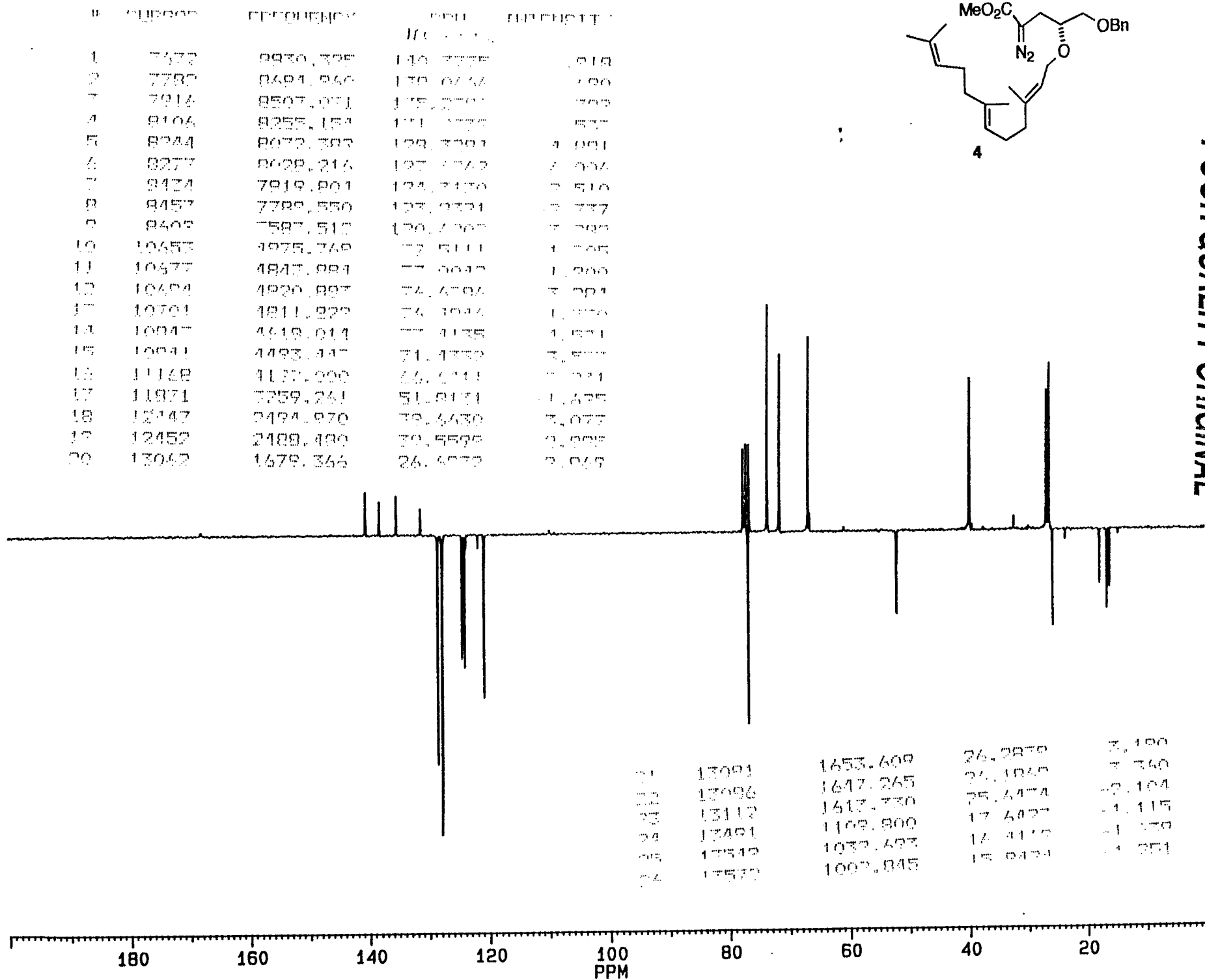
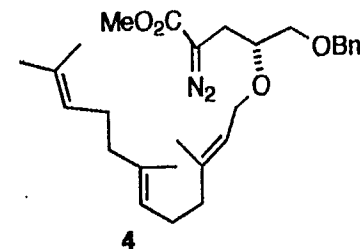
3b

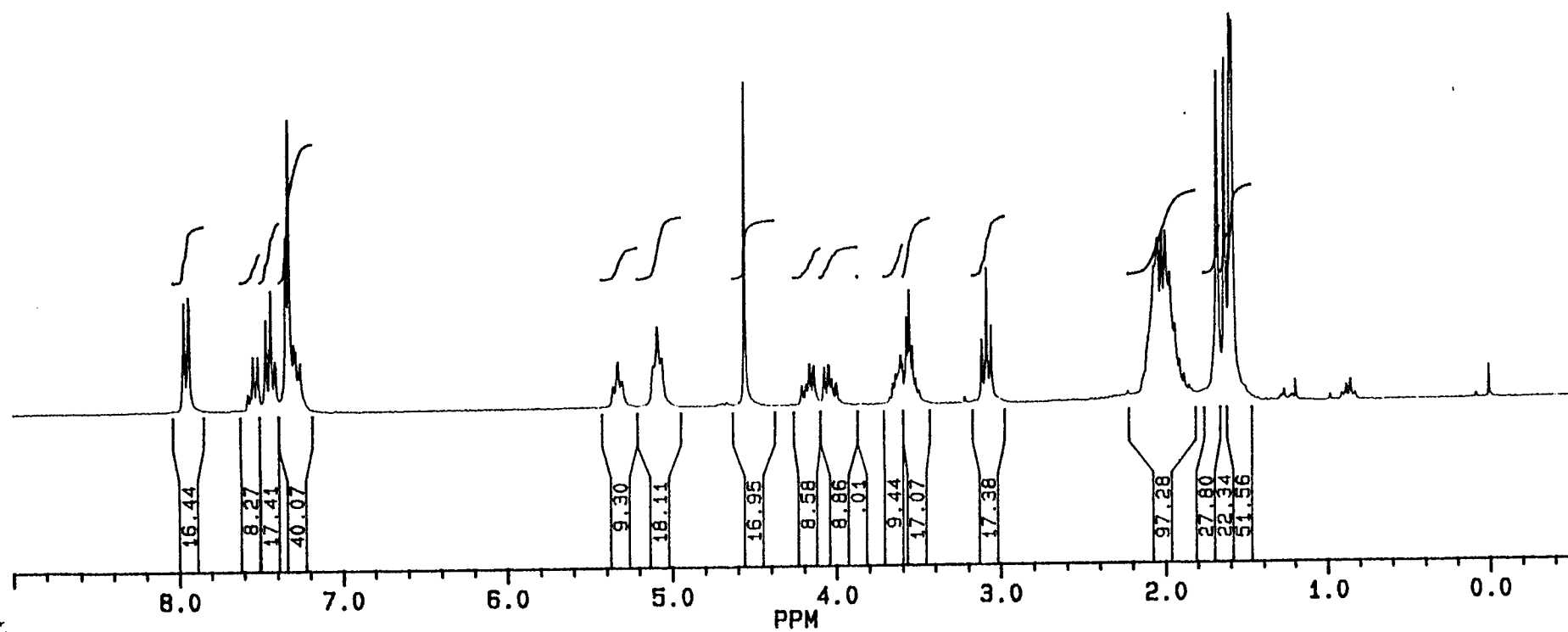
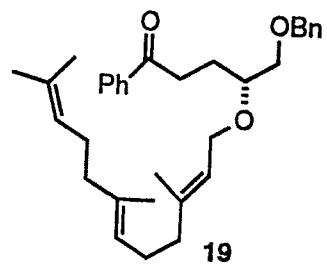




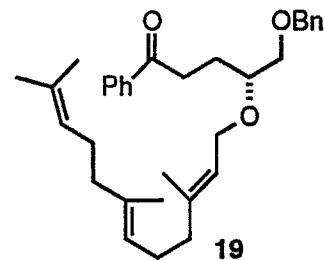


POOR QUALITY ORIGINAL

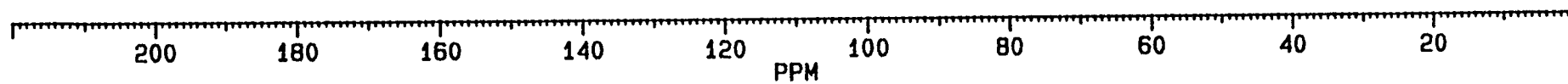
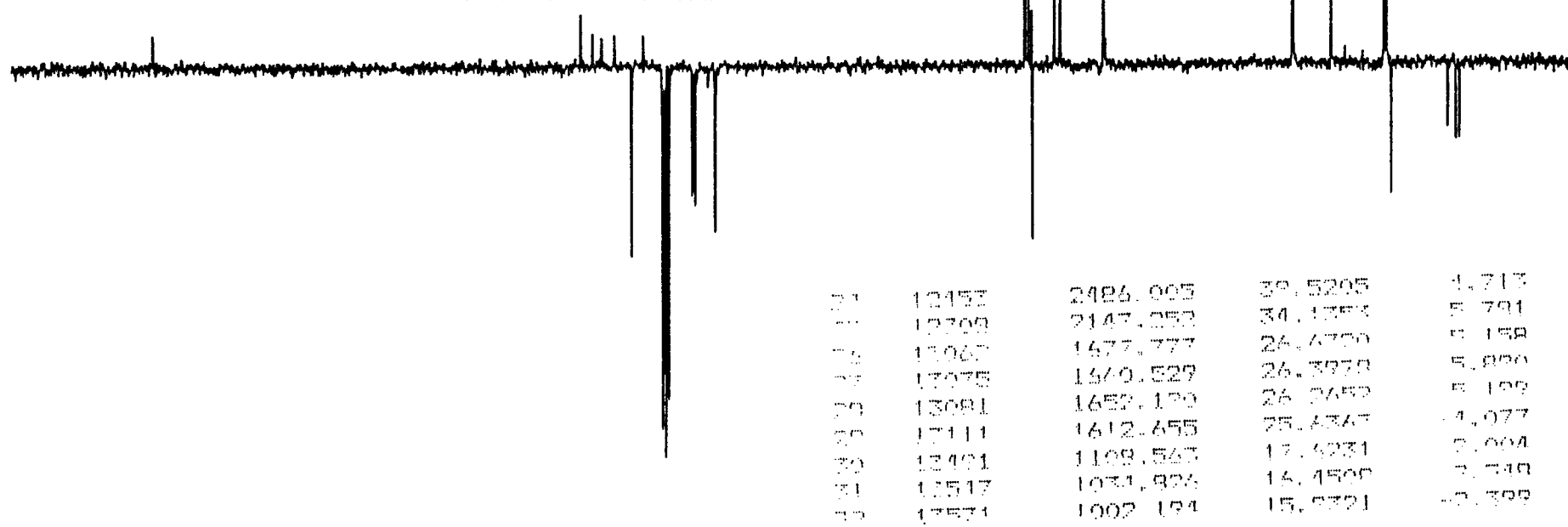


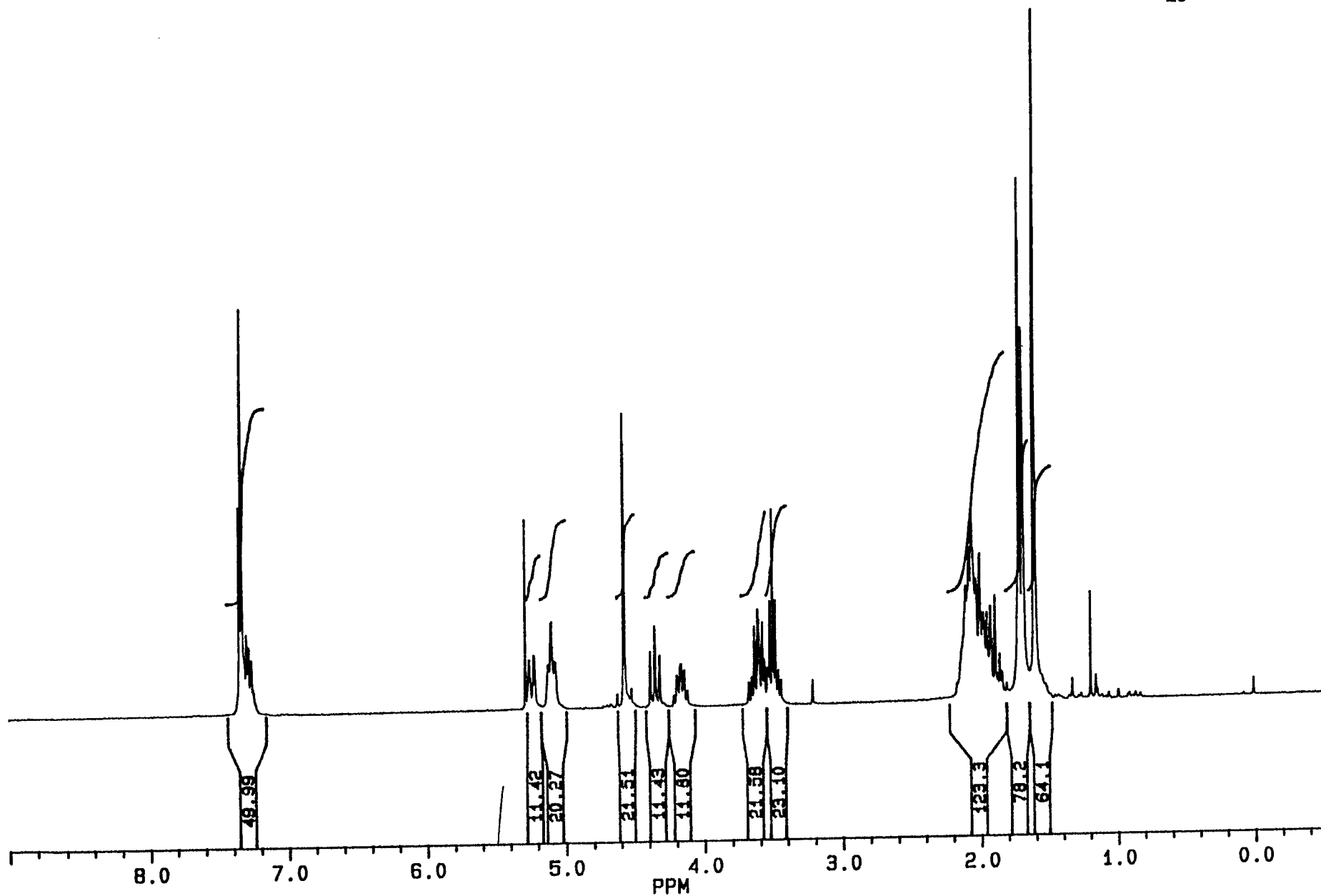
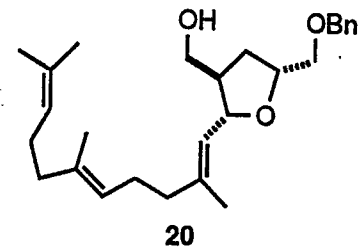


POOR QUALITY ORIGINAL

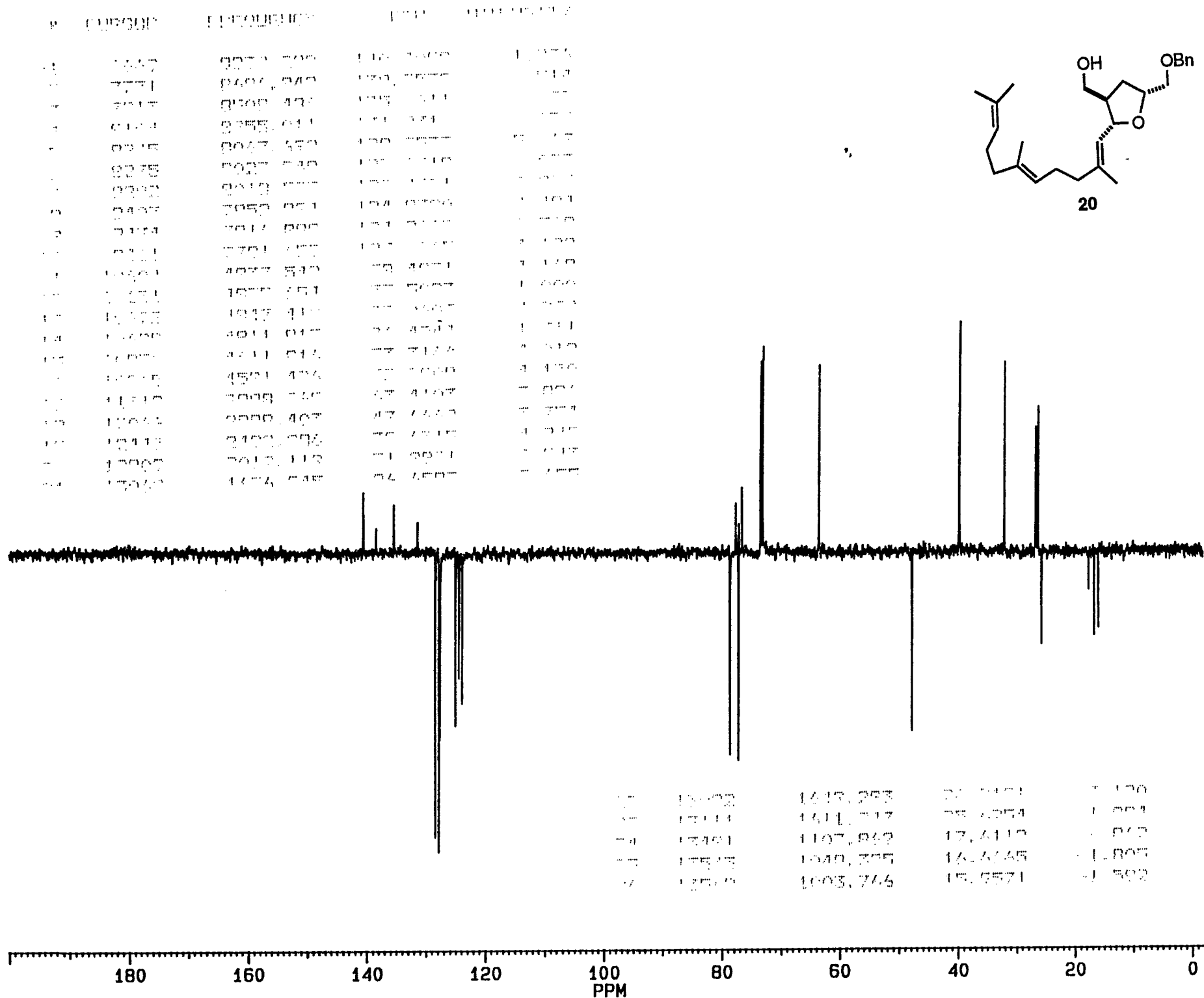
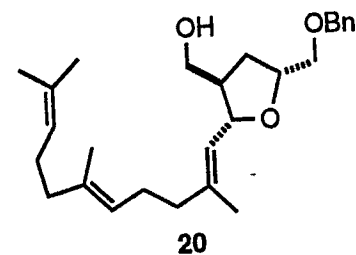


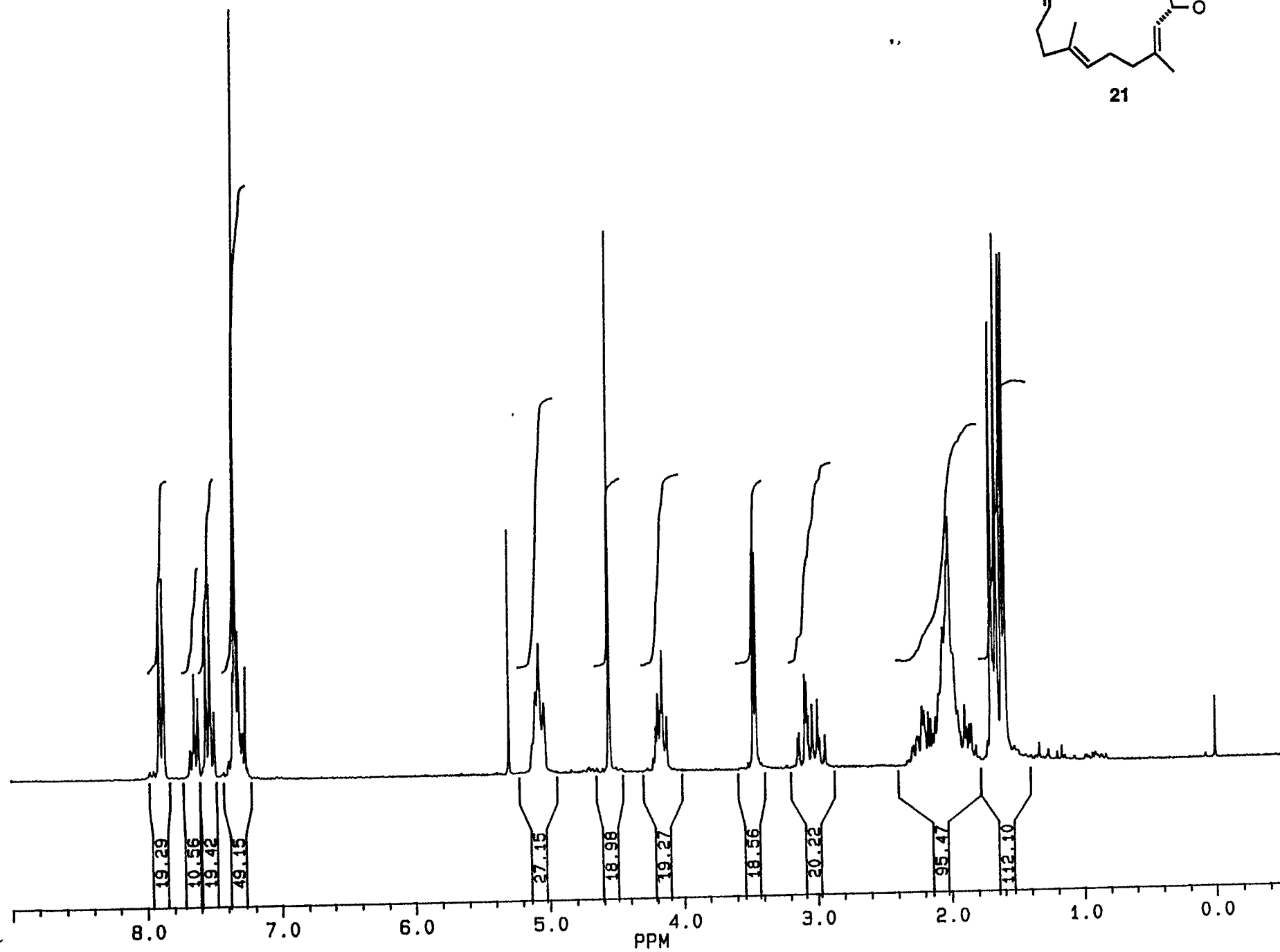
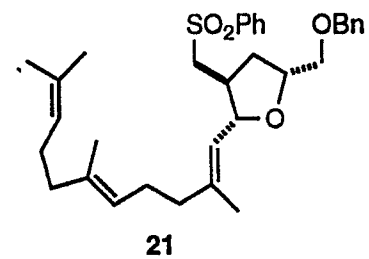
1	4842	12594.080	200.0517	4.044
2	7691	8904.361	137.2647	1.470
3	7772	8674.894	139.2579	1.054
4	7937	8617.258	134.0207	1.039
5	7919	8502.370	135.1437	1.099
6	9070	8354.488	132.9142	5.070
7	8104	8253.780	131.3130	0.000
8	8236	8080.736	129.4411	-11.551
9	8244	8070.143	128.7847	0.570
10	8258	8051.585	127.9277	-12.551
11	8277	8024.513	127.5881	-10.757
12	8381	8020.812	127.5085	-4.102
13	8474	7818.028	124.2840	-4.128
14	8455	7790.018	123.9395	-4.528
15	8588	7614.405	121.0477	-5.183
16	10652	4875.179	77.5017	2.711
17	10674	4843.377	76.9261	1.955
18	10700	4811.770	76.4269	1.790
19	10703	4807.937	76.4312	-5.375
20	10851	4611.599	73.3115	7.195
21	10898	4562.330	72.5283	5.274
22	11179	4176.058	66.3876	6.009
23	12447	2493.406	39.4414	5.296



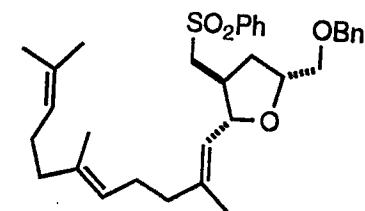


POOR QUALITY ORIGINAL

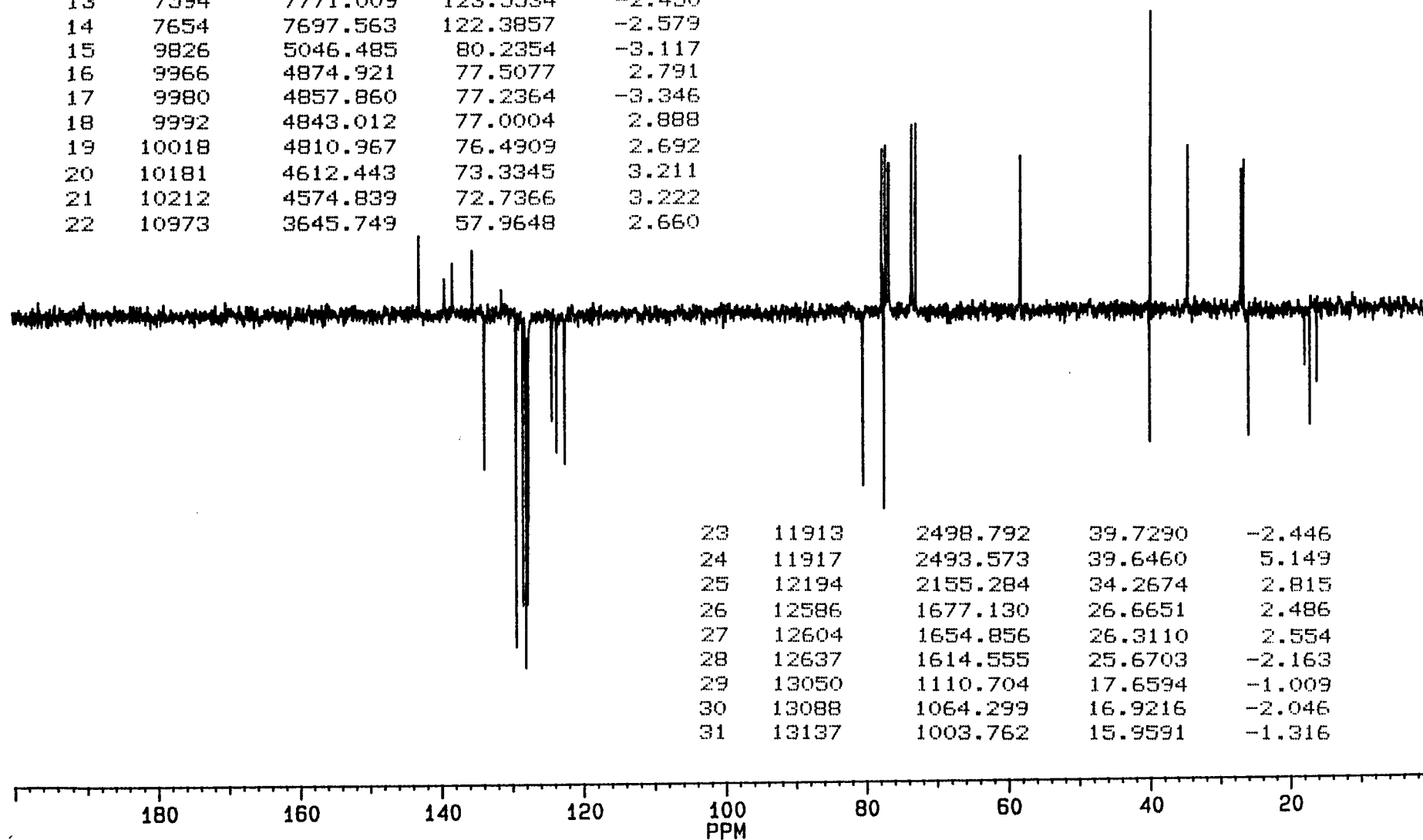


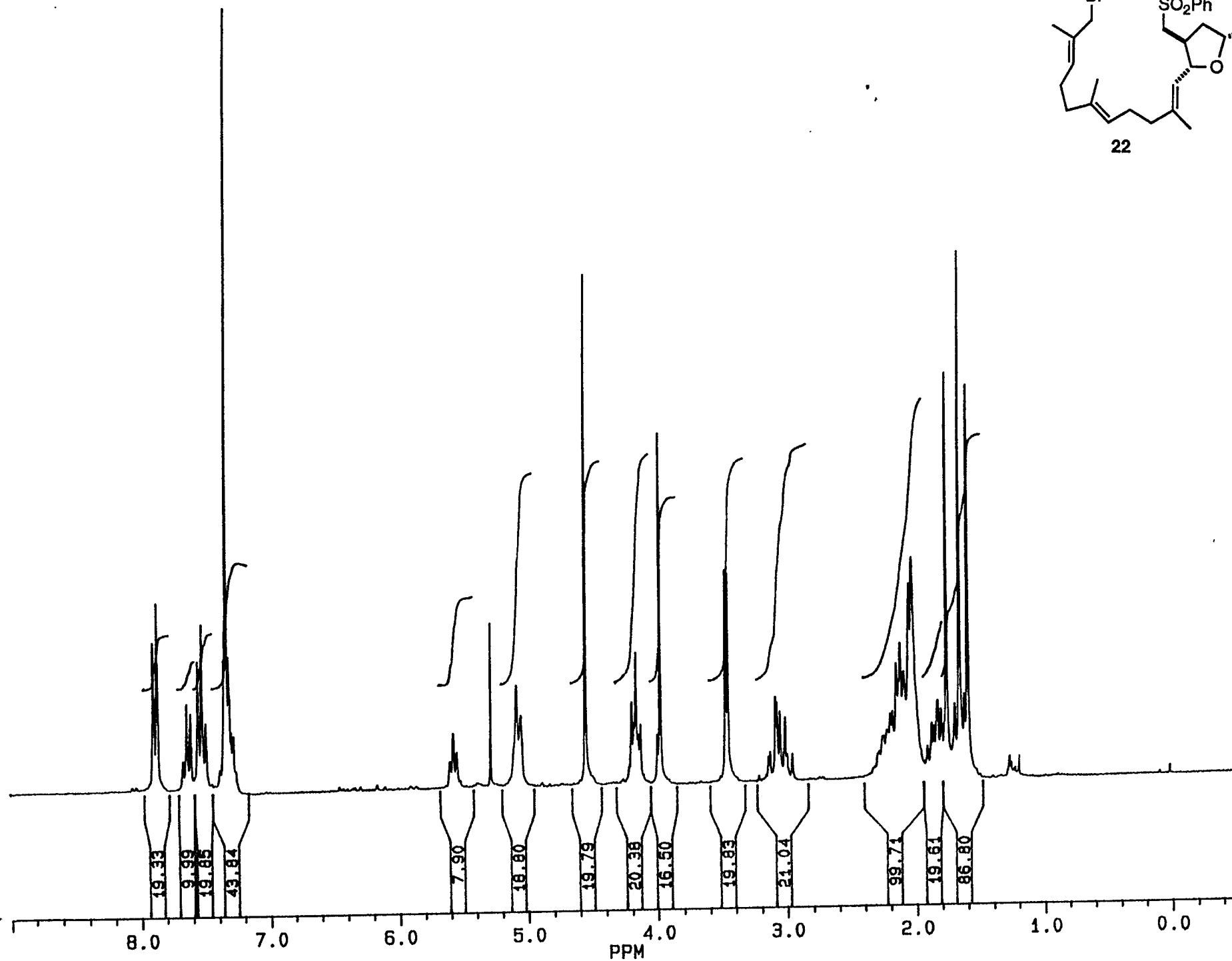
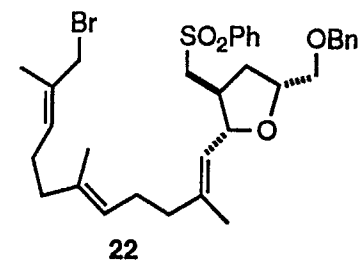


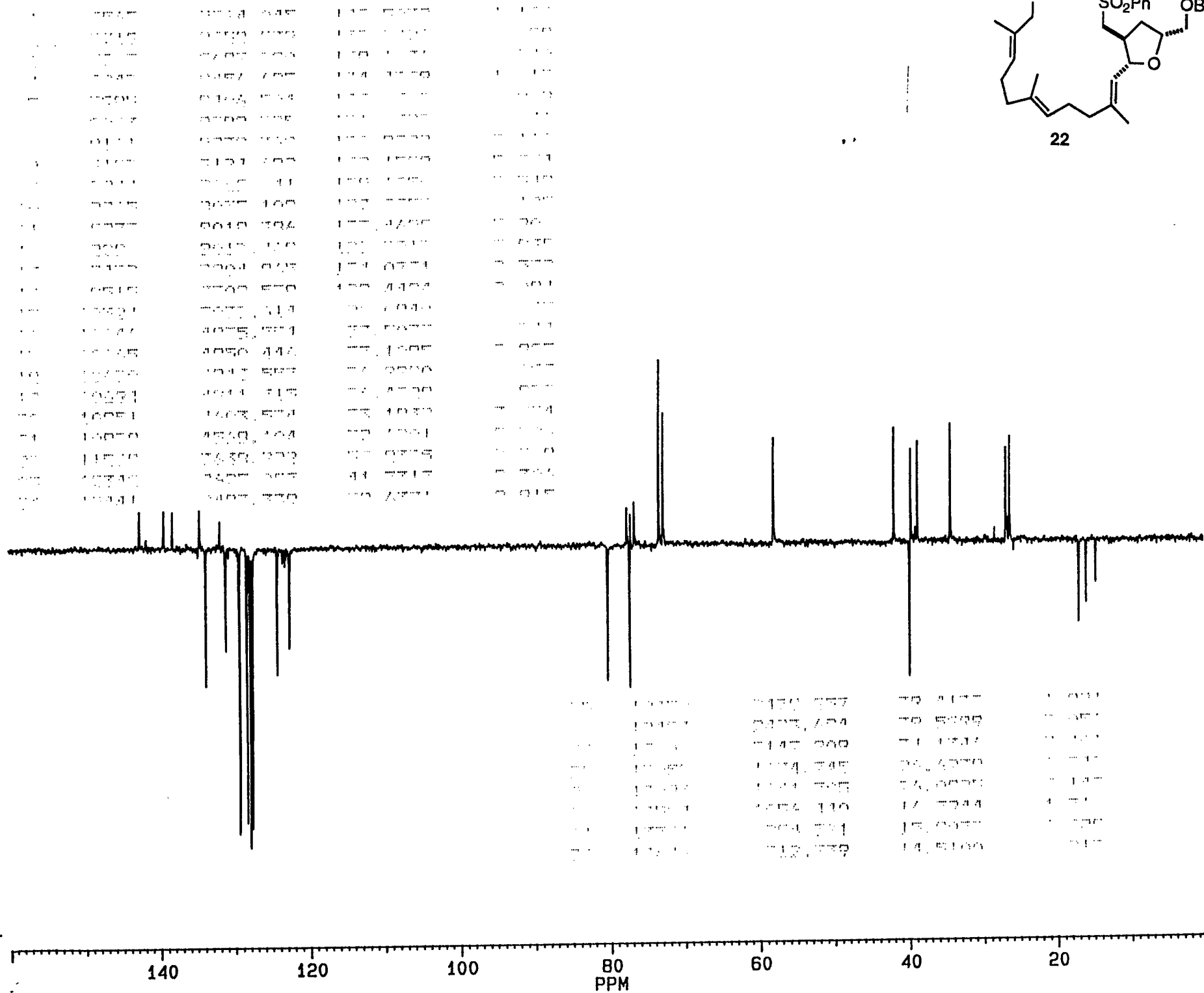
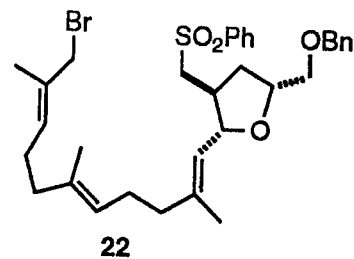
#	CURSOR	FREQUENCY	PPM	INTENSITY
1	6596	8989.045	142.9193	1.398
2	6781	8763.480	139.3330	.663
3	6839	8691.980	138.1962	.894
4	6983	8516.402	135.4046	1.097
5	7068	8412.172	133.7474	-2.742
6	7194	8258.281	131.3007	.464
7	7299	8130.365	129.2669	-5.755
8	7349	8069.721	128.3027	-4.970
9	7371	8042.879	127.8759	-6.029
10	7384	8026.538	127.6161	-5.072
11	7389	8020.707	127.5234	-3.534
12	7559	7813.555	124.2298	-1.837
13	7594	7771.009	123.5534	-2.450
14	7654	7697.563	122.3857	-2.579
15	9826	5046.485	80.2354	-3.117
16	9966	4874.921	77.5077	2.791
17	9980	4857.860	77.2364	-3.346
18	9992	4843.012	77.0004	2.888
19	10018	4810.967	76.4909	2.692
20	10181	4612.443	73.3345	3.211
21	10212	4574.839	72.7366	3.222
22	10973	3645.749	57.9648	2.660



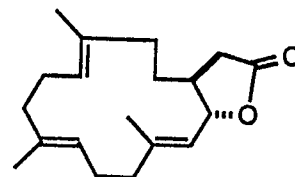
21



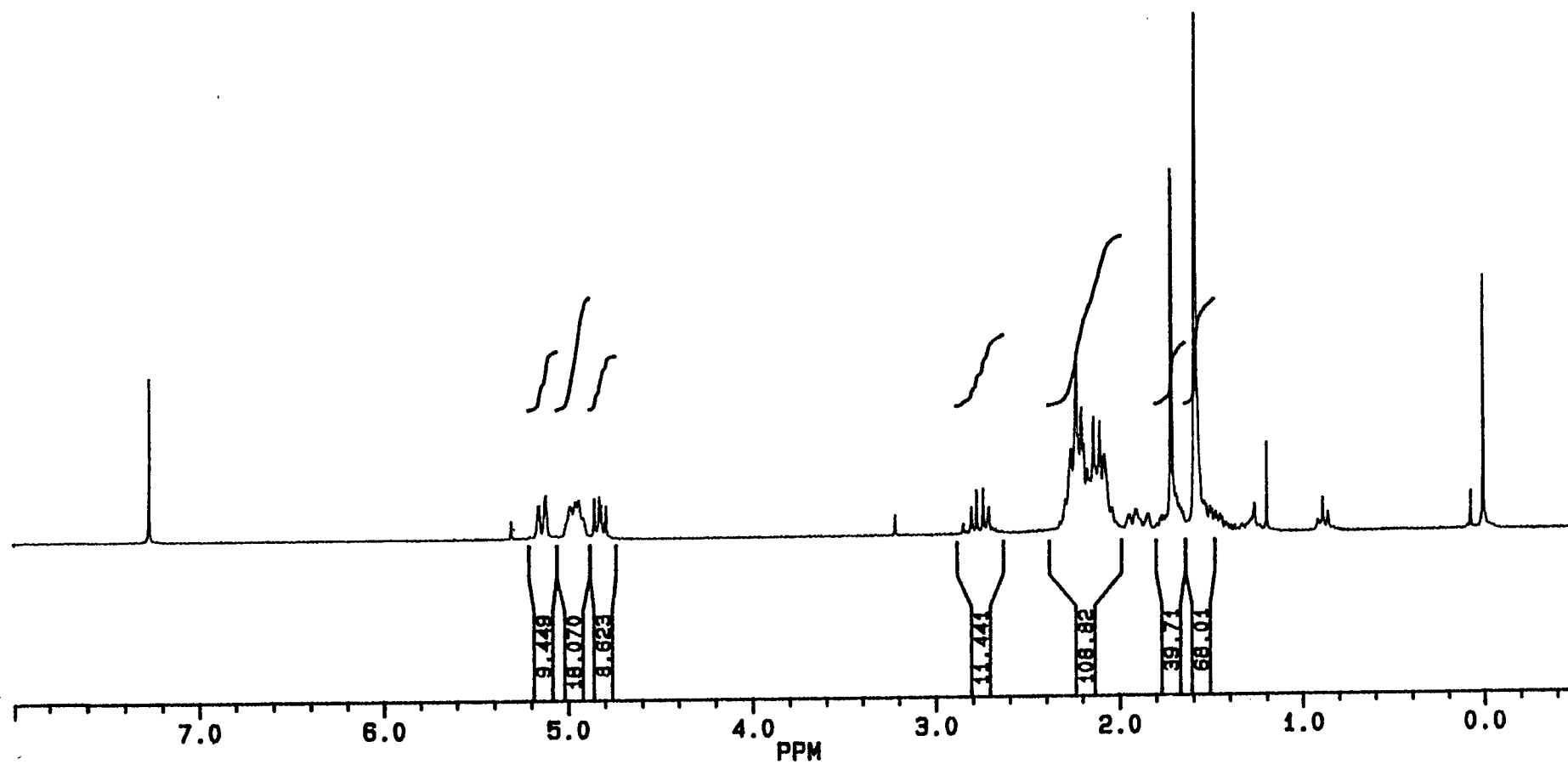




POOR QUALITY ORIGINAL

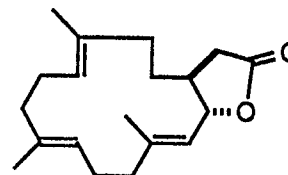


23



#	ADDRESS	FREQUENCY [Hz]	PPM	INTENSITY
1	8821.9	17841.592	177.3294	1.28
2	13175.3	14231.396	141.4473	2.09
3	14039.3	13514.872	134.3257	2.11
4	14278.9	13316.167	132.3507	2.56
5	15060.6	12667.926	125.9078	-5.52
6	15354.8	12423.957	123.4830	-5.44
7	15388.2	12396.259	123.2077	-5.72
8	20399.6	8240.364	81.9018	-5.88
9	20904.3	7821.876	77.7424	48.58
10	20942.9	7789.859	77.4242	50.00
11	20981.3	7757.985	77.1074	49.64
12	25426.4	4071.799	40.4700	-5.27
13	25556.1	3964.225	39.4008	4.10
14	25563.0	3958.514	39.3441	5.09
15	25627.0	3905.378	38.8159	4.97
16	25929.3	3654.731	36.3247	5.30
17	26063.0	3543.867	35.2228	4.78
18	26677.0	3034.655	30.1617	4.57
19	27171.1	2624.945	26.0896	3.97
20	27351.9	2475.020	24.5995	4.34

e



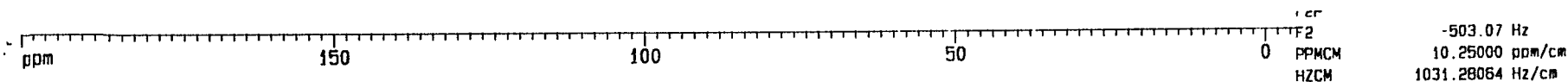
23

rent Data Parameters
 E lactone
 NO 1
 JCNO 1

- Acquisition Parameters
 te_ 960923.
 ime 21.09
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG jvert
 TD 65536
 SOLVENT CDCl3
 NS 6084
 DS 0
 SWH 27173.912 Hz
 FIDRES 0.414641 Hz
 AQ 1.2059124 sec
 RG 2048
 DM 18.400 usec
 DE 4.50 usec
 TE 300.0 K
 D11 0.03000000 sec
 PL12 18.00 dB
 D1 6.00000000 sec
 CPDPRG2 waltz16
 PCPD2 95.00 usec
 SF02 400.1320007 MHz
 NUC2 1H
 PL2 120.00 dB
 D13 0.00000300 sec
 P1 10.50 usec
 D20 0.00700000 sec
 P2 21.00 usec
 DE 4.50 usec
 SF01 100.6242995 MHz
 NUC1 13C
 PL1 0.00 dB

F2 - Processing parameters

21	27418.0	2420.186	24.0545	4.67
22	27454.2	2390.130	23.7557	3.96
23	28166.5	1799.411	17.8845	-2.13
24	28250.1	1730.097	17.1956	-3.06
25	28439.0	1573.460	15.6388	-2.99
26	28571.0	1464.003	14.5509	-3.37
27	30162.7	144.027	1.4315	-1.05
28	30287.1	40.876	0.4063	-1.75



CF
 F2 -503.07 Hz
 PPMCM 10.25000 ppm/cm
 HZCM 1031.28054 Hz/cm