
1,7-Antarafacial H Shift Transition State **44** to **45**

AM1 Heat of Formation: -34.950 kcal/mol
B3LYP/6-31G*//AM1 SCF total energy: -960.5951152 hartrees
One Imaginary Mode -2105 cm -1

		Cartesian Coordinates (Angstroms)		
Atom		X	Y	Z
1	C C1	-0.0240170	0.6484293	1.3320792
2	C C2	-1.1829860	0.5436415	2.1088072
3	H H5	-2.1267286	0.7698398	1.5632402
4	C C3	1.2506967	0.1308571	1.5803690
5	C C4	1.6314843	-0.8847637	2.4898521
6	H H2	2.7241473	-1.0876091	2.5866533
7	C C5	-1.3609462	0.2799051	3.4555714
8	H H8	-2.4079193	0.1309839	3.7904242
9	C C6	-0.3559676	0.1572088	4.4313616
10	H H10	0.5710106	0.7571127	4.2602677
11	O O1	0.8520431	-1.6502746	3.1662705
12	H H6	0.1817051	-1.0301065	4.0300353
13	C C7	2.3974875	0.6035424	0.7642858
14	C C8	-0.2555774	1.4295290	0.0645060
15	O O2	3.5308459	0.7583630	1.2301687
16	O O3	-1.2383241	2.1664100	-0.0614490
17	C C9	2.1269422	0.8800914	-0.6783217
18	H H1	3.0099797	1.1589622	-1.2865424
19	C C10	0.7456036	1.3171123	-1.0483360
20	C C11	-0.7450625	0.0483053	5.8719019
21	H H3	0.1806323	0.1091849	6.5048086
22	H H9	-1.3949386	0.9199431	6.1551920
23	C C12	-1.4720301	-1.2449852	6.1807985
24	H H13	-0.8194889	-2.1171547	5.9101049
25	H H14	-2.3985830	-1.3184131	5.5523278
26	C C13	-1.8464389	-1.3259658	7.6455181
27	H H7	-0.9182356	-1.2580619	8.2725180
28	H H17	-2.4920960	-0.4488866	7.9159868
29	C C14	-2.5756055	-2.6071280	7.9576365
30	H H15	-1.9392756	-3.4924360	7.7151152
31	H H18	-3.5177909	-2.6802043	7.3623471
32	H H19	-2.8393924	-2.6484695	9.0419403
33	O O4	1.2099079	-0.0195612	-1.3176514
34	C C15	0.4909179	2.1536196	-2.2736403
35	H H12	-0.5850961	2.0159722	-2.5760806
36	H H16	1.1330465	1.7720672	-3.1129194
37	C C16	0.7352976	3.5954082	-2.0193737
38	H H20	0.1476113	4.0189836	-1.1861502
39	C C17	1.5631122	4.3442562	-2.7432917
40	H H11	1.7012484	5.4158505	-2.5474520
41	H H21	2.1542512	3.9461713	-3.5788563

Syn Trienol Precursor to Cyclohexanol **45**

Heat of Formation: -70.481 kcal/mol
B3LYP/6-31G*//AM1 -960.61150

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 C C1	0.0141471	-0.1012246	0.8916913
2 C C3	1.2826396	-0.7332066	1.2227306
3 C C4	1.4038177	-1.9298492	1.8564538
4 H H2	2.3839678	-2.3959251	2.0809648
5 C C6	-0.0539414	0.1775106	4.0150326
6 H H10	0.9175078	0.5377388	3.6272342
7 O O1	0.3958558	-2.7283884	2.2759398
8 C C7	2.5151142	-0.0624969	0.7774263
9 C C8	-0.1376798	0.3393213	-0.5194007
10 O O2	3.5898760	-0.1544341	1.3806208
11 O O3	-1.2009801	0.2564720	-1.1377247
12 C C9	2.4135670	0.7500558	-0.4765768
13 H H1	3.2449835	1.4683422	-0.6286171
14 C C10	1.0874327	0.9587325	-1.1354645
15 C C11	-0.1010202	0.0313992	5.4864094
16 H H3	0.7271214	-0.6660367	5.7964406
17 H H9	0.1294125	1.0328093	5.9467247
18 C C12	-1.4141061	-0.4798566	6.0387065
19 H H13	-1.6516920	-1.4796410	5.5885729
20 H H14	-2.2436584	0.2202994	5.7552071
21 C C13	-1.3559382	-0.6076241	7.5470227
22 H H7	-0.5235960	-1.3046831	7.8316006
23 H H17	-1.1183286	0.3921564	7.9979248
24 C C14	-2.6583804	-1.1191820	8.1071202
25 H H15	-2.8986878	-2.1267682	7.6896358
26 H H18	-3.4967632	-0.4260889	7.8535573
27 H H19	-2.5953095	-1.2044401	9.2188014
28 O O4	2.0426991	0.0144040	-1.6544394
29 C C15	0.8344314	2.1526360	-2.0168927
30 H H16	1.7420041	2.3359001	-2.6532807
31 C C16	0.4793318	3.3585400	-1.2290652
32 H H20	-0.3240985	3.2101966	-0.4878717
33 C C17	1.0487460	4.5484765	-1.4033456
34 H H11	0.7458646	5.4305358	-0.8239361
35 H H21	1.8488196	4.7261278	-2.1336256
36 C C2	-1.0605819	-0.0812520	3.1685315
37 H H8	-2.0431016	-0.4258737	3.5398874
38 C C5	-1.0094735	0.1368680	1.7397302
39 H H23	-1.9438621	0.5620021	1.3170215
40 H H4	-0.0195674	1.9006136	-2.7079389
41 H H5	-0.4606517	-2.2983189	2.1053237

Anti-Trienol - Precursor to Cyclohexanol **46**

AM1 Heat of Formation: -72.571 kcal/mol
B3LYP/6-31G*//AM1 SCF total energy: -960.6153555 hartrees

		Cartesian Coordinates (Angstroms)		
	Atom	X	Y	Z
1	C C1	-0.0682310	0.0034489	0.9325019
2	C C3	1.1782765	-0.7005404	1.2089765
3	C C4	1.1437080	-2.0438189	1.4507730
4	H H2	0.2032505	-2.6317793	1.4179231
5	C C6	-1.0891775	-1.0775625	3.8498390
6	H H10	-0.4467132	-0.2246931	4.1344604
7	O O1	2.1791807	-2.8546191	1.7437258
8	C C7	2.4349142	0.0475332	1.2033821
9	C C8	-0.0351675	1.0782405	-0.0902111
10	O O2	3.4738927	-0.3811028	1.7316014
11	O O3	-0.9874694	1.3193123	-0.8363119
12	C C9	2.4498958	1.3817595	0.5256454
13	H H1	3.2498473	2.0649241	0.8777744
14	C C10	1.2161169	1.9110406	-0.1277249
15	C C11	-1.3983295	-1.9960605	4.9689941
16	H H3	-0.4269729	-2.3879370	5.3818754
17	H H9	-1.8834160	-1.3992919	5.7911498
18	C C12	-2.2926830	-3.1631938	4.6098779
19	H H13	-1.8133508	-3.7739047	3.7998467
20	H H14	-3.2692391	-2.7835519	4.2085658
21	C C13	-2.5506296	-4.0415115	5.8165906
22	H H7	-1.5739370	-4.4215062	6.2181880
23	H H17	-3.0264158	-3.4305482	6.6289532
24	C C14	-3.4427598	-5.2053944	5.4700172
25	H H15	-2.9729182	-5.8417822	4.6815313
26	H H18	-4.4293569	-4.8468599	5.0885195
27	H H19	-3.6225624	-5.8378768	6.3726224
28	O O4	2.2901236	1.3426914	-0.9022132
29	C C15	1.0074469	3.3889539	-0.3237524
30	H H16	1.9718913	3.8513978	-0.6679578
31	C C16	0.5068954	4.0471969	0.9082020
32	H H20	-0.3668043	3.5612736	1.3742718
33	C C17	1.0334972	5.1582556	1.4170272
34	H H11	0.6244127	5.6395048	2.3150329
35	H H21	1.9012396	5.6650491	0.9740001
36	C C2	-1.5173440	-1.2098077	2.5896831
37	H H8	-2.1748270	-2.0452571	2.2854650
38	C C5	-1.2502390	-0.2542034	1.5310368
39	H H23	-2.1490611	0.2996187	1.1891047
40	H H4	0.2512824	3.5278725	-1.1480548
41	H H5	3.0205506	-2.3631396	1.7854802

Cyclohexanol Product Forming Transition State **46** to **42**

AM1 Heat of Formation: -38.567 kcal/mol
B3LYP/6-31G*//AM1: SCF total energy: -960.5750051 hartrees

One imaginary mode -745 cm -1

	Cartesian Coordinates (Angstroms)		
Atom	X	Y	Z
1 C C1	-1.1608100	-0.7299854	0.8003663
2 C C3	0.1787628	-0.9172428	0.4200526
3 C C7	0.6072916	-2.2391112	-0.0688618
4 C C8	-1.9520218	-1.8578818	1.3516622
5 O O2	1.4164882	-2.4217395	-0.9810644
6 O O3	-3.0892290	-1.6970792	1.8070226
7 C C9	-0.0170529	-3.4077471	0.6313072
8 H H1	0.2863016	-4.4000238	0.2403203
9 C C10	-1.3224910	-3.2238250	1.3385328
10 O O4	-0.0802124	-3.3227815	2.0627415
11 C C15	-2.2607178	-4.3844222	1.5393218
12 H H16	-1.6601208	-5.3014007	1.7842934
13 C C16	-3.1248267	-4.6062462	0.3535213
14 H H20	-3.6905984	-3.7173998	0.0251191
15 C C17	-3.2506574	-5.7794059	-0.2612129
16 H H11	-3.9198490	-5.9187717	-1.1203764
17 H H21	-2.7015701	-6.6783426	0.0490198
18 H H4	-2.9148571	-4.1561005	2.4277437
19 C C2	-1.8696987	0.4279135	0.4719772
20 H H3	-2.9688488	0.3994659	0.5951643
21 C C4	-1.3015483	1.5055623	-0.2009474
22 H H5	-1.9080153	1.9759112	-0.9977343
23 C C5	1.0954930	0.1609023	0.3913217
24 H H7	1.3515987	0.6415442	1.3550685
25 C C6	0.0045964	1.9471558	0.0016517
26 H H10	0.2847336	2.1995375	1.0426186
27 O O1	2.0963113	0.0872416	-0.5441625
28 H H6	2.7975369	0.6986199	-0.2748736
29 C C11	0.7051578	2.7237611	-1.0552382
30 H H2	1.2155401	1.9968798	-1.7493550
31 H H12	-0.0343404	3.3007523	-1.6741391
32 C C12	1.7353272	3.6751429	-0.4806162
33 H H14	1.2424387	4.3801368	0.2393591
34 C C18	2.4227615	4.4661516	-1.5730356
35 H H17	2.8904875	3.7600069	-2.3093545
36 H H23	1.6589336	5.0681336	-2.1330678
37 C C19	3.4768834	5.3838483	-1.0097723
38 H H9	4.2687733	4.7990625	-0.4817275
39 H H24	3.0278599	6.1015721	-0.2811936
40 H H25	3.9589907	5.9689442	-1.8298044
41 H H26	2.4997325	3.0912606	0.0983521

Cyclohexanol Product **42**

AM1 Heat of Formation: -82.360 kcal/mol
B3LYP/6-31G*//AM1 SCF total energy: -960.6318299 hartrees

		Cartesian Coordinates (Angstroms)		
	Atom	X	Y	Z
1	C C1	0.1427365	-0.3218413	0.6908890
2	C C3	1.3964758	-0.6760192	1.0680782
3	C C7	2.5746546	-0.4136571	0.2183831
4	C C8	-0.1573624	0.3748694	-0.5836000
5	O O2	3.6692247	-0.9579106	0.3942354
6	O O3	-1.2988693	0.4618389	-1.0398448
7	C C9	2.3912922	0.5818926	-0.8862845
8	H H1	3.2684104	1.2378224	-1.0612094
9	C C10	1.0156548	1.0002912	-1.2878462
10	O O4	1.7827760	0.0714020	-2.0822578
11	C C15	0.7553665	2.3318986	-1.9377378
12	H H16	1.5735599	2.5426239	-2.6783489
13	C C16	0.6414416	3.4225610	-0.9379658
14	H H20	-0.0732299	3.2316758	-0.1195878
15	C C17	1.3142120	4.5679211	-1.0163724
16	H H11	1.1882487	5.3697913	-0.2768753
17	H H21	2.0294797	4.7871777	-1.8208476
18	H H4	-0.2115471	2.2570221	-2.5120162
19	C C2	-0.9920667	-0.6162664	1.5493770
20	H H3	-1.9939486	-0.4801218	1.1097194
21	C C4	-0.8083768	-1.0194811	2.8157959
22	H H5	-1.6601191	-1.2115181	3.4870496
23	C C5	1.6102448	-1.4512170	2.3454274
24	H H7	1.5501155	-2.5454430	2.0572056
25	C C6	0.5424264	-1.1802364	3.4244973
26	H H10	0.5286108	-2.0950982	4.0857298
27	O O1	2.8687727	-1.1861903	2.9375130
28	H H6	3.5450730	-1.6083863	2.3892063
29	C C11	0.8567895	0.0360639	4.2947195
30	H H2	1.4542713	0.7727909	3.6968881
31	H H12	-0.1006854	0.5397360	4.5943338
32	C C12	1.6287658	-0.3449504	5.5406597
33	H H14	1.0320406	-1.0736302	6.1499444
34	C C18	1.9444348	0.8752326	6.3798003
35	H H17	2.5562691	1.5948794	5.7743611
36	H H23	0.9913303	1.4002932	6.6530686
37	C C19	2.6943011	0.5032258	7.6327197
38	H H9	3.6536756	-0.0095220	7.3797845
39	H H24	2.0859778	-0.1860503	8.2666940
40	H H25	2.9292464	1.4167199	8.2303548
41	H H26	2.5826708	-0.8563692	5.2421642

[4+2] Transition State to **3**

Heat of Formation: -119.003 kcal/mol
B3LYP/6-31G*//AM1 SCF total energy: -1921.2635588 hartrees

Imaginary Mode -757.62

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 C C1	-1.0139438	-2.9502854	-0.4800060
2 C C2	-2.2595764	-2.8164976	0.0607700
3 H H6	-2.9767249	-3.6475265	0.1966477
4 C C3	-0.6433681	-4.2550435	-1.0367628
5 O O1	-1.3500591	-5.2634763	-0.9093102
6 C C5	-0.6250012	-0.5657988	-0.0470876
7 H H10	-0.1677317	0.3497396	-0.4889394
8 C C6	-2.1138391	-0.4270380	0.1593845
9 O O2	-2.7751213	-1.6538351	0.5408289
10 C C7	0.6103271	-4.3205002	-1.8487706
11 H H9	0.6394899	-5.1631633	-2.5710752
12 C C8	1.4340545	-3.0931487	-2.0739516
13 O O3	1.8374095	-4.1143528	-1.1363045
14 C C9	1.0161137	-1.7896017	-1.4460902
15 O O4	1.6116610	-0.7429178	-1.7474441
16 C C10	2.3128965	-2.9819865	-3.2925270
17 H H4	2.8056318	-3.9739940	-3.4796559
18 H H7	3.1255579	-2.2332517	-3.0721118
19 C C11	-2.7669133	0.1187374	-1.1119776
20 H H11	-2.1843344	1.0106335	-1.4623418
21 H H14	-2.7171379	-0.6611892	-1.9157820
22 C C4	-0.1259234	-1.8051671	-0.5297829
23 C C12	1.3222517	-2.5014242	1.3552952
24 H H15	1.6643628	-3.4908521	0.9870827
25 C C15	0.0466697	-0.1929872	1.7411312
26 H H12	-0.4950020	0.7513244	1.9435039
27 O O5	0.2190475	-2.6067025	2.1231460
28 C C16	-0.4054072	-1.3687631	2.5638226
29 C C14	2.0999208	-1.3325036	1.2853916
30 C C17	1.4353849	-0.1143531	1.4837245
31 C C18	3.5219940	-1.4026785	0.9321373
32 C C19	2.0807748	1.1895973	1.2394925
33 C C20	4.2918257	-0.1227472	1.0507144
34 H H23	5.3112077	-0.1662515	0.6131417
35 C C21	3.5823919	1.1909448	1.1972336
36 O O6	4.2164197	0.5436201	2.3178750
37 O O7	4.0858272	-2.4394743	0.5707358
38 O O8	1.4204512	2.2174947	1.0582950
39 C C22	-0.0928737	-1.1985848	4.0483841
40 H H5	0.9414431	-0.7849026	4.1733039
41 H H19	-0.1111982	-2.2111877	4.5331053
42 C C23	4.2371901	2.4535493	0.7030034
43 H H16	3.7484308	2.7326509	-0.2719368
44 H H20	5.3225880	2.2459609	0.5005671

45	C	C13	1.5497486	-2.5246592	-4.4802473
46	H	H18	0.9654388	-1.6015779	-4.3234044
47	C	C24	1.5789769	-3.1398616	-5.6594888
48	C	C28	-4.2069655	0.5114318	-0.8634386
49	H	H24	-4.2478987	1.3310615	-0.0981721
50	H	H29	-4.7637683	-0.3663958	-0.4401049
51	C	C29	-4.8729593	0.9752417	-2.1409748
52	H	H13	-4.3025311	1.8403928	-2.5709662
53	H	H32	-4.8458009	0.1503823	-2.9010812
54	C	C30	-6.3084439	1.3877471	-1.8926165
55	H	H30	-6.3338438	2.2143397	-1.1340259
56	H	H33	-6.8754869	0.5228317	-1.4572115
57	C	C31	-6.9785229	1.8451371	-3.1624230
58	H	H31	-6.4399399	2.7203780	-3.5996784
59	H	H35	-8.0337264	2.1471644	-2.9568559
60	H	H36	-6.9876956	1.0255525	-3.9211491
61	C	C33	-1.1022288	-0.2914437	4.7170720
62	H	H39	-2.1332779	-0.7187132	4.5992268
63	H	H40	-1.0986559	0.7132358	4.2170433
64	C	C34	-0.7879461	-0.1257543	6.1888152
65	H	H2	0.2431290	0.3002722	6.3082591
66	H	H41	-0.7914513	-1.1298303	6.6894559
67	C	C35	-1.7932446	0.7820291	6.8653263
68	H	H43	-2.8246072	0.3582435	6.7387036
69	H	H44	-1.7853727	1.7866393	6.3653296
70	C	C36	-1.4891740	0.9443069	8.3322636
71	H	H42	-0.4734774	1.3854821	8.4782385
72	H	H45	-1.5196994	-0.0432433	8.8531679
73	H	H46	-2.2391073	1.6190571	8.8111688
74	C	C37	4.0879600	3.5842021	1.6536286
75	C	C38	5.1096519	4.3025524	2.1118915
76	H	H1	-2.3564090	0.2535459	1.0270557
77	H	H3	-1.5071704	-1.5698499	2.4203626
78	H	H37	3.0458780	3.8045879	1.9438294
79	H	H22	2.1573079	-4.0553547	-5.8408831
80	H	H27	1.0255568	-2.7615007	-6.5288234
81	H	H38	4.9655688	5.1486616	2.7964874
82	H	H47	6.1538359	4.0989892	1.8402415

[4+2] Transition State to **33**

AM1 Heat of Formation: -118.6 kcal/mol

B3LYP/6-31G* SCF total energy: -1921.2628702 hartrees
-767.43 cm -1

Cartesian Coordinates (Angstroms)

Atom			X	Y	Z
1	O	O1	-8.9495896	0.9978396	-7.2253378
2	O	O2	-8.8953344	-3.0464100	-6.2296449
3	O	O3	-10.4393994	0.4153009	-2.3909164
4	O	O4	-11.6737298	-2.1851408	-4.3336059

5	C	C1	-8.6704241	-0.2333924	-6.7387284
6	C	C2	-9.3453040	-0.7867179	-5.6355238
7	C	C3	-9.4683715	-2.2403792	-5.4879326
8	C	C4	-10.3421808	-2.7189152	-4.3708120
9	C	C5	-10.7715124	-1.7787077	-3.2863046
10	C	C6	-10.3402382	-0.3394677	-3.3631453
11	C	C7	-9.7894241	0.1101661	-4.6537804
12	C	C8	-9.5164507	1.4760493	-4.8916490
13	C	C9	-9.6113474	1.9263407	-6.3240913
14	C	C10	-11.0651159	2.0759434	-6.7650620
15	C	C11	-11.1631359	2.7559655	-8.1130786
16	C	C12	-12.6021525	2.8478846	-8.5728890
17	C	C13	-12.7049343	3.5374367	-9.9168888
18	C	C14	-14.1352673	3.6287495	-10.3820467
19	C	C15	-11.0769376	-2.2579497	-1.8936537
20	C	C16	-11.5661775	-3.6567360	-1.8437417
21	C	C17	-11.1817909	-4.5374743	-0.9230739
22	O	O7	-6.9148344	3.4644739	-5.9152910
23	O	O8	-5.1388243	0.8376121	-8.6359737
24	O	O9	-6.8563549	-1.1068843	-3.8185985
25	C	C20	-6.2763279	2.5953947	-6.7426746
26	C	C21	-6.2071460	1.2477534	-6.5507717
27	C	C22	-5.4337375	0.4426567	-7.5013291
28	C	C23	-4.9984825	-0.9097978	-7.0377395
29	C	C24	-5.5176294	-1.4823306	-5.7557472
30	C	C25	-6.4652316	-0.6710982	-4.9112282
31	C	C26	-6.8838333	0.6447545	-5.4179091
32	C	C27	-7.5728131	1.5126618	-4.5295261
33	C	C28	-7.2845263	2.9909484	-4.6007456
34	C	C29	-6.1726170	3.3503448	-3.6127507
35	C	C30	-6.0309080	4.8499500	-3.4692993
36	C	C31	-4.8799091	5.2019415	-2.5516652
37	C	C32	-4.7428752	6.7015823	-2.3946147
38	C	C33	-3.5951024	7.0582698	-1.4858109
39	H	H1	-8.0868491	-0.8291490	-7.4646602
40	H	H2	-10.2791203	-3.8102730	-4.1745420
41	H	H3	-9.8489083	2.2157640	-4.1399040
42	H	H4	-9.0531475	2.8934254	-6.4909978
43	H	H5	-11.5467002	1.0644635	-6.8115780
44	H	H6	-11.6079104	2.6788920	-5.9908459
45	H	H7	-10.5591576	2.1797651	-8.8635205
46	H	H8	-10.7205189	3.7851258	-8.0506353
47	H	H9	-13.0412526	1.8178697	-8.6450476
48	H	H10	-13.2055397	3.4122880	-7.8138065
49	H	H11	-12.2657676	4.5675015	-9.8432170
50	H	H12	-12.0974518	2.9732143	-10.6732137
51	H	H13	-14.1884667	4.1395905	-11.3736354
52	H	H14	-14.7513424	4.2087187	-9.6529146
53	H	H15	-14.5823519	2.6104100	-10.4854583
54	H	H16	-10.1461491	-2.1292827	-1.2764801
55	H	H17	-11.8632670	-1.5793193	-1.4567190
56	H	H18	-12.3069991	-3.9165822	-2.6197931
57	H	H22	-5.8479970	3.1286877	-7.6117823
58	H	H24	-7.7002691	1.1477839	-3.4853719
59	H	H25	-8.2026381	3.6080399	-4.3739486
60	H	H26	-6.4133311	2.8938850	-2.6171306

61	H	H27	-5.2058820	2.9075162	-3.9683322
62	H	H28	-6.9830649	5.2821625	-3.0624372
63	H	H29	-5.8648244	5.3060113	-4.4813428
64	H	H30	-5.0421838	4.7320233	-1.5458462
65	H	H31	-3.9260850	4.7790751	-2.9643508
66	H	H32	-5.6968778	7.1228551	-1.9802908
67	H	H33	-4.5857098	7.1696902	-3.4023152
68	H	H34	-3.5118302	8.1671401	-1.3833886
69	H	H35	-2.6318047	6.6684830	-1.8952494
70	H	H36	-3.7456721	6.6203926	-0.4694108
71	H	H43	-10.4462808	-4.3024594	-0.1421422
72	H	H47	-11.5833954	-5.5588307	-0.8899828
73	H	H37	-4.6337971	-1.5746838	-7.8487330
74	O	O5	-4.1908095	-0.9283567	-5.8520217
75	C	C18	-5.5951624	-2.9788581	-5.5944649
76	H	H19	-5.0755665	-3.4658479	-6.4637146
77	H	H20	-6.6818001	-3.2755399	-5.6354350
78	C	C19	-5.0158297	-3.4497854	-4.3114189
79	H	H38	-5.3514836	-2.8899922	-3.4208934
80	C	C34	-4.1753973	-4.4770789	-4.2181043
81	H	H23	-3.7805751	-4.8197015	-3.2528660
82	H	H39	-3.8236883	-5.0439662	-5.0900034

[4+2] Dimer **32**

Heat of Formation: -166.440 kcal/mol
B3LYP/6-31G*//AM1 -1921.3058355 hartrees

		Cartesian Coordinates (Angstroms)		
Atom		X	Y	Z
1	O	O1	8.8826678	7.1611105	-0.9357511
2	O	O2	8.7149864	6.1431596	2.9187365
3	O	O3	11.2778162	2.8542869	-0.6359770
4	O	O4	11.7042110	4.6996910	2.1827644
5	C	C1	8.1385729	6.3771475	-0.0010761
6	C	C2	9.0903514	5.4201641	0.6776241
7	C	C3	9.3219430	5.4205091	2.1279611
8	C	C4	10.3570420	4.4455995	2.6078775
9	C	C5	11.0575415	3.5255613	1.6547695
10	C	C6	10.7446733	3.6065793	0.1821098
11	C	C7	9.7494598	4.6205486	-0.1950003
12	C	C8	9.3495229	4.8616014	-1.6230882
13	C	C9	9.5636811	6.3609100	-1.9210349
14	C	C10	11.0362875	6.7434252	-1.9358466
15	C	C11	11.2272206	8.1607917	-2.4308736
16	C	C12	12.6874828	8.5569855	-2.4008507
17	C	C13	12.8823347	9.9717723	-2.9032716
18	C	C14	14.3346372	10.3725869	-2.8757475
19	C	C15	11.5984244	2.1912604	2.0908640
20	C	C16	11.9877348	2.1494637	3.5209401
21	C	C17	11.7407761	1.1144861	4.3203042
22	O	O7	7.0256687	5.7924635	-3.7150225
23	O	O8	4.8093860	8.4119895	-1.3596060

24	O	O9	6.2684728	3.5575046	0.3464834
25	O	O10	5.6670371	6.8255612	1.5357222
26	C	C20	6.2882826	6.6040018	-2.9128336
27	C	C21	6.1981567	6.4897372	-1.5644771
28	C	C22	5.2525122	7.3685393	-0.8658129
29	C	C23	4.7322781	6.8884066	0.4538076
30	C	C24	5.1918088	5.5726885	1.0059059
31	C	C25	6.1943923	4.7808213	0.2124702
32	C	C26	7.0598851	5.5448959	-0.7889061
33	C	C27	7.8357722	4.5614149	-1.7080160
34	C	C28	7.3726022	4.5085849	-3.1609566
35	C	C29	6.1985196	3.5481272	-3.3392175
36	C	C30	5.8885033	3.3213496	-4.8029324
37	C	C31	4.6860992	2.4178216	-4.9712992
38	C	C32	4.3747554	2.1865412	-6.4347090
39	C	C33	3.1804549	1.2841739	-6.6086130
40	C	C34	4.2801395	4.7830872	1.9089481
41	C	C35	4.9980358	4.1650714	3.0518583
42	C	C36	4.6706913	4.3661499	4.3255151
43	H	H1	7.6761330	7.1192093	0.7035051
44	H	H2	10.2618328	4.1716143	3.6802832
45	H	H3	9.9323725	4.2223293	-2.3321040
46	H	H4	9.0836906	6.6157384	-2.9089598
47	H	H5	11.4589227	6.6448457	-0.9019916
48	H	H6	11.5839506	6.0274044	-2.6028221
49	H	H7	10.6279628	8.8587389	-1.7874869
50	H	H8	10.8326531	8.2518515	-3.4771656
51	H	H9	13.0784865	8.4741907	-1.3524731
52	H	H10	13.2843197	7.8481674	-3.0334049
53	H	H11	12.4881137	10.0542126	-3.9506913
54	H	H12	12.2837358	10.6782201	-2.2691598
55	H	H13	14.4556567	11.4182814	-3.2484817
56	H	H14	14.9436033	9.6949804	-3.5220667
57	H	H15	14.7386673	10.3198246	-1.8356898
58	H	H16	10.8218959	1.4127156	1.8587974
59	H	H17	12.5030746	1.9607424	1.4589386
60	H	H18	12.5340640	3.0397247	3.8783733
61	H	H22	5.7822498	7.3903169	-3.5058641
62	H	H23	3.7423133	7.3081804	0.7303311
63	H	H24	7.6994545	3.5154833	-1.2989261
64	H	H25	8.2282746	4.1895448	-3.8266752
65	H	H26	6.4520988	2.5705778	-2.8513141
66	H	H27	5.2981534	3.9655503	-2.8175038
67	H	H28	6.7784865	2.8629271	-5.3097323
68	H	H29	5.6966608	4.3088757	-5.3007572
69	H	H30	4.8804467	1.4338659	-4.4682672
70	H	H31	3.7954894	2.8769214	-4.4664709
71	H	H32	5.2679437	1.7316421	-6.9394617
72	H	H33	4.1793747	3.1719139	-6.9353031
73	H	H34	2.9666688	1.1291973	-7.6936135
74	H	H35	2.2749536	1.7311092	-6.1311368
75	H	H36	3.3670679	0.2875395	-6.1398777
76	H	H37	3.4604385	5.4583906	2.2754243
77	H	H38	3.8112689	3.9668102	1.2923599
78	H	H39	5.8281383	3.4974086	2.7641325
79	H	H43	11.2010038	0.2178432	3.9875227

80	H	H47	12.0690653	1.0961002	5.3679627
81	H	H50	5.2086239	3.8781026	5.1488350
82	H	H52	3.8533152	5.0305346	4.6354824

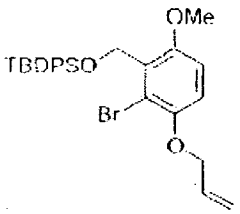
[4+2] Dimer **33** AM1 optimized geometry

Heat of Formation: -167.865 kcal/mol
B3LYP/6-31G*//AM1 = -1921.3032431 hartrees

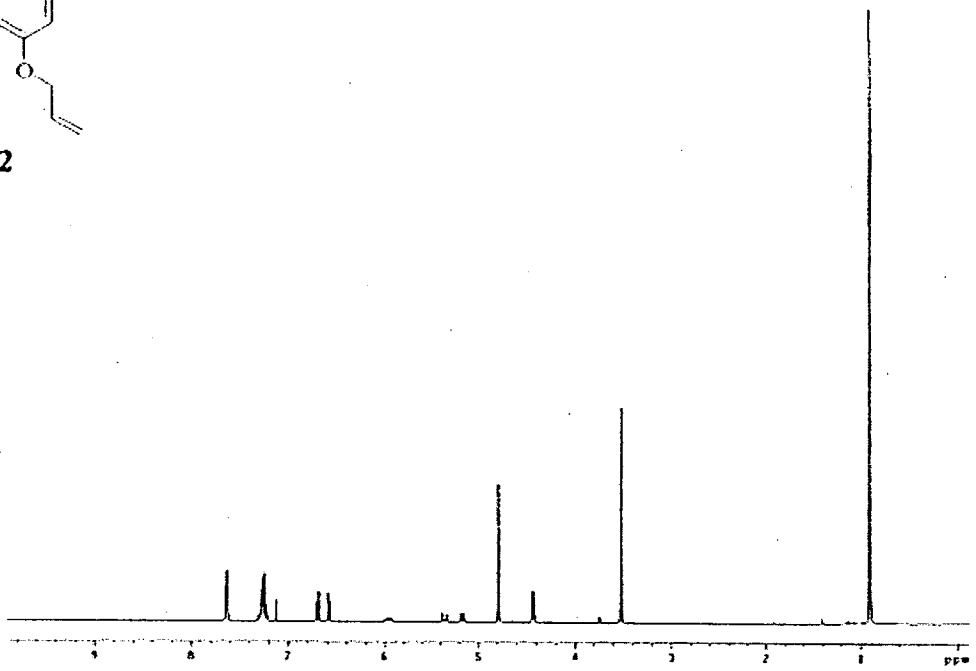
Cartesian Coordinates (Angstroms)

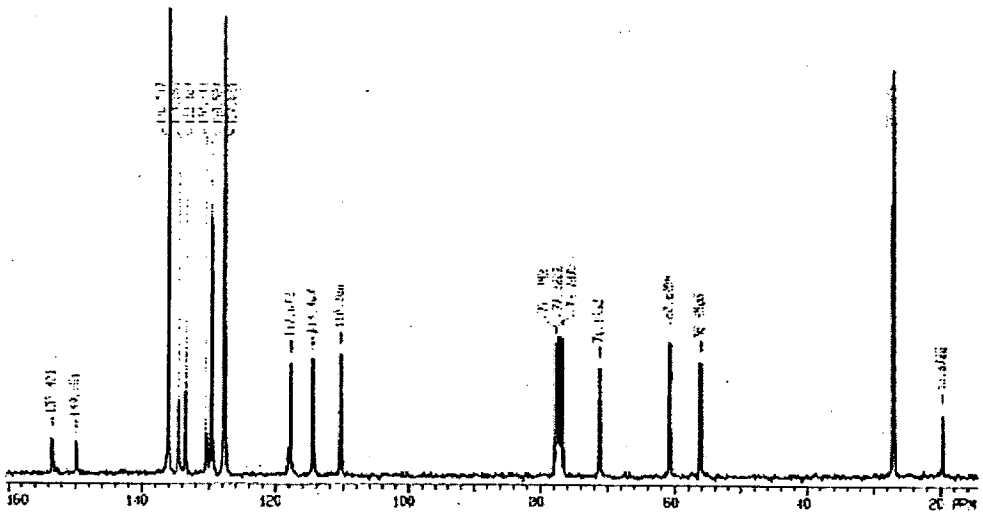
Atom		X	Y	Z
1	O	O1	8.9559458	7.1703914	-0.8954598
2	O	O2	8.6844813	6.0512158	2.9425651
3	O	O3	11.2337679	2.8016978	-0.6458865
4	O	O4	11.7246502	4.6927353	2.1456822
5	C	C1	8.1814488	6.3937983	0.0212278
6	C	C2	9.1065934	5.4044098	0.6897843
7	C	C3	9.3303117	5.3738653	2.1396857
8	C	C4	10.3922726	4.4229281	2.6050023
9	C	C5	11.0828835	3.5060037	1.6405950
10	C	C6	10.7347241	3.5734182	0.1749332
11	C	C7	9.7518132	4.6040947	-0.1929578
12	C	C8	9.3504805	4.8642956	-1.6176332
13	C	C9	9.5940004	6.3620303	-1.9045659
14	C	C10	11.0743527	6.7106702	-1.9460953
15	C	C11	11.2878907	8.1258491	-2.4382696
16	C	C12	12.7567662	8.4899856	-2.4315728
17	C	C13	12.9737954	9.9014749	-2.9346707
18	C	C14	14.4336687	10.2741711	-2.9214815
19	C	C15	11.6512316	2.1820074	2.0732687
20	C	C16	12.0615937	2.1524199	3.4977051
21	C	C17	11.8216255	1.1265825	4.3108388
22	O	O7	7.0373165	5.8091276	-3.7163028
23	O	O8	5.0958259	8.6476979	-1.3361276
24	O	O9	6.1258711	3.6731682	0.3173147
25	C	C20	6.3489147	6.6710827	-2.9223119
26	C	C21	6.2801019	6.5949503	-1.5713512
27	C	C22	5.4281083	7.5568337	-0.8601497
28	C	C23	4.9412503	7.1429508	0.4947468
29	C	C24	5.3125851	5.8046857	1.0496785
30	C	C25	6.1689571	4.8978216	0.2066357
31	C	C26	7.0859918	5.6086901	-0.7865892
32	C	C27	7.8300683	4.5940395	-1.6918667
33	C	C28	7.3483143	4.5268378	-3.1380847
34	C	C29	6.1395966	3.6039429	-3.2805108
35	C	C30	5.8150585	3.3427447	-4.7354120
36	C	C31	4.5694335	2.4938760	-4.8709982
37	C	C32	4.2553819	2.2096259	-6.3245752
38	C	C33	3.0099183	1.3735008	-6.4664461
39	H	H1	7.7298000	7.1331299	0.7321457
40	H	H2	10.3258531	4.1552841	3.6812916
41	H	H3	9.9158356	4.2193464	-2.3354341
42	H	H4	9.0978903	6.6369263	-2.8790781

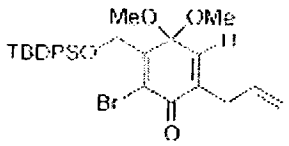
43	H	H5	11.5147419	6.5969961	-0.9212736
44	H	H6	11.5921933	5.9859567	-2.6273671
45	H	H7	10.7152245	8.8339908	-1.7820085
46	H	H8	10.8775991	8.2301347	-3.4772520
47	H	H9	13.1632125	8.3963190	-1.3898640
48	H	H10	13.3275459	7.7697365	-3.0753918
49	H	H11	12.5707374	9.9925349	-3.9780319
50	H	H12	12.3953877	10.6187364	-2.2940469
51	H	H13	14.5713375	11.3165881	-3.2978423
52	H	H14	15.0233712	9.5834902	-3.5717987
53	H	H15	14.8462040	10.2159725	-1.8850585
54	H	H16	10.8837934	1.3905319	1.8549936
55	H	H17	12.5499871	1.9634831	1.4289269
56	H	H18	12.6175011	3.0435987	3.8377874
57	H	H22	5.8712097	7.4664859	-3.5262899
58	H	H24	7.6694262	3.5596940	-1.2618336
59	H	H25	8.1851014	4.1650234	-3.8056593
60	H	H26	6.3593026	2.6336678	-2.7625585
61	H	H27	5.2574268	4.0698032	-2.7680491
62	H	H28	6.6801443	2.8245142	-5.2272703
63	H	H29	5.6695103	4.3207535	-5.2663343
64	H	H30	4.7106453	1.5262819	-4.3208848
65	H	H31	3.7006835	3.0207999	-4.3951311
66	H	H32	5.1227931	1.6772768	-6.7972041
67	H	H33	4.1238123	3.1787980	-6.8746520
68	H	H34	2.7982409	1.1728973	-7.5443181
69	H	H35	2.1290240	1.9000908	-6.0260326
70	H	H36	3.1299299	0.3946476	-5.9423978
71	H	H43	11.2724196	0.2293669	3.9951806
72	H	H47	12.1657502	1.1168863	5.3535214
73	H	H37	4.6664937	7.9850124	1.1627758
74	O	O5	4.0050345	6.0527860	0.4995496
75	C	C18	5.3773663	5.5943702	2.5386898
76	H	H19	4.8908978	6.4707968	3.0477175
77	H	H20	6.4618991	5.5880046	2.8442381
78	C	C19	4.7397030	4.3266343	2.9736407
79	H	H38	4.8732896	3.4733431	2.2856124
80	C	C34	4.0634241	4.2045406	4.1131290
81	H	H23	3.6169576	3.2513478	4.4250179
82	H	H39	3.9074525	5.0395254	4.8087756



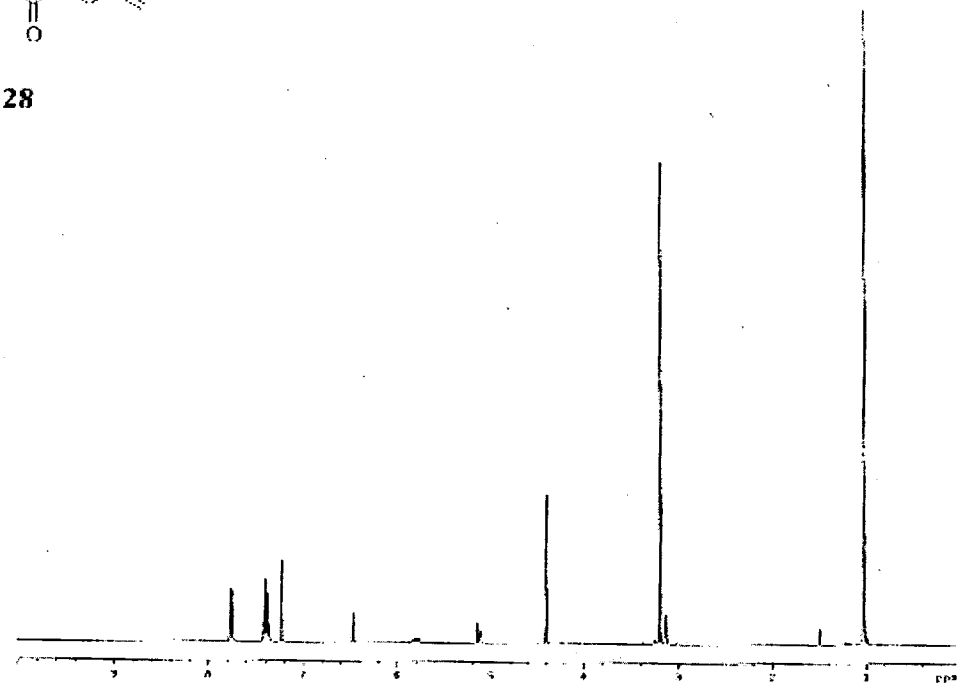
12

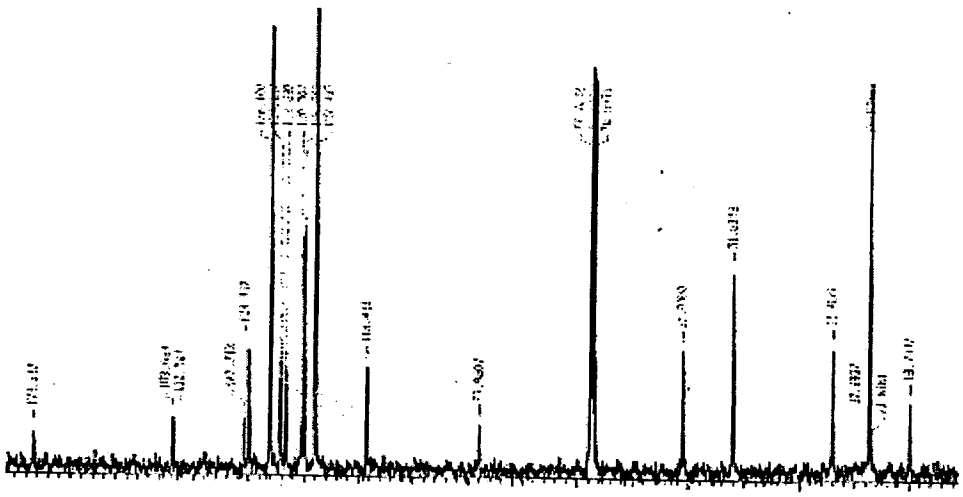


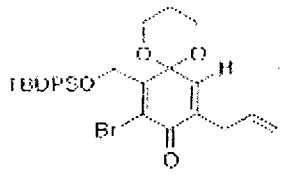




28







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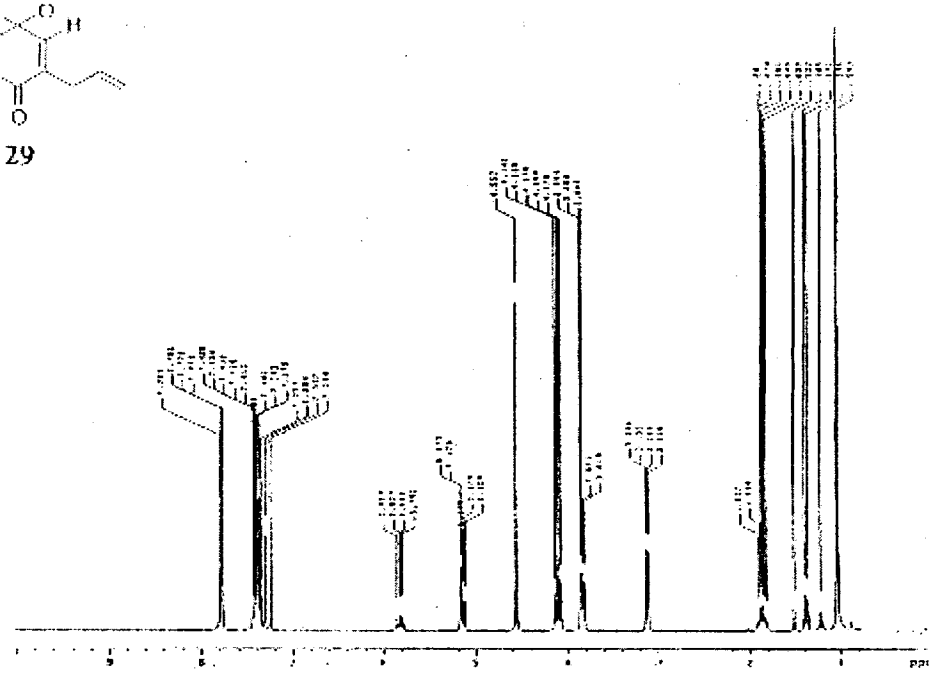

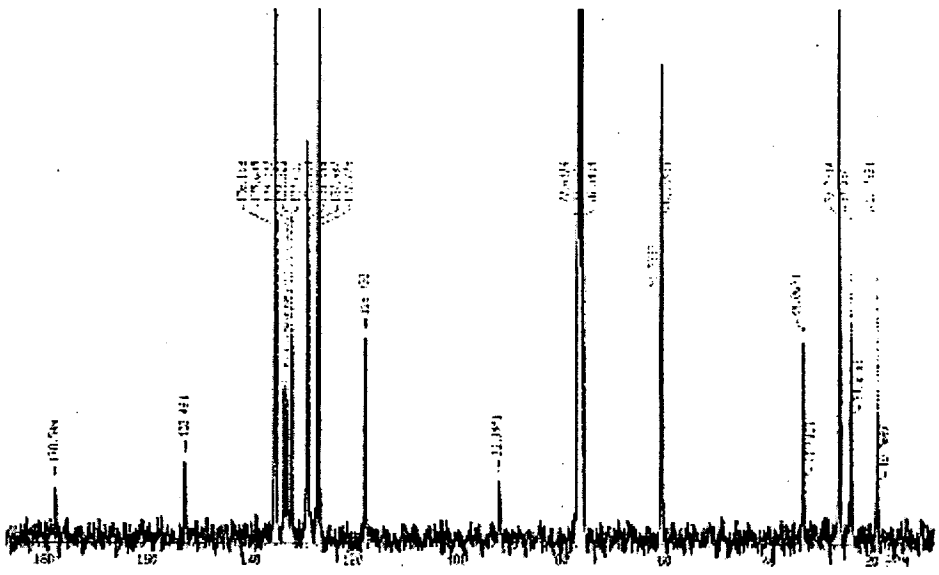

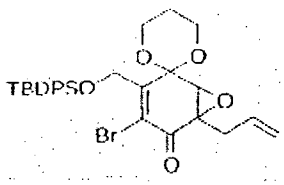

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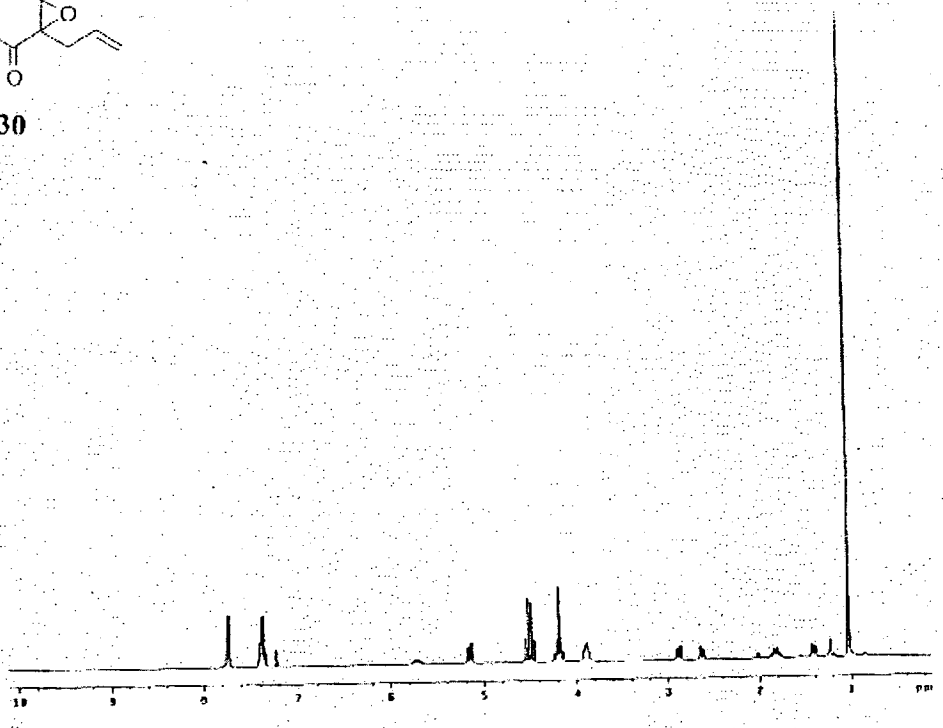

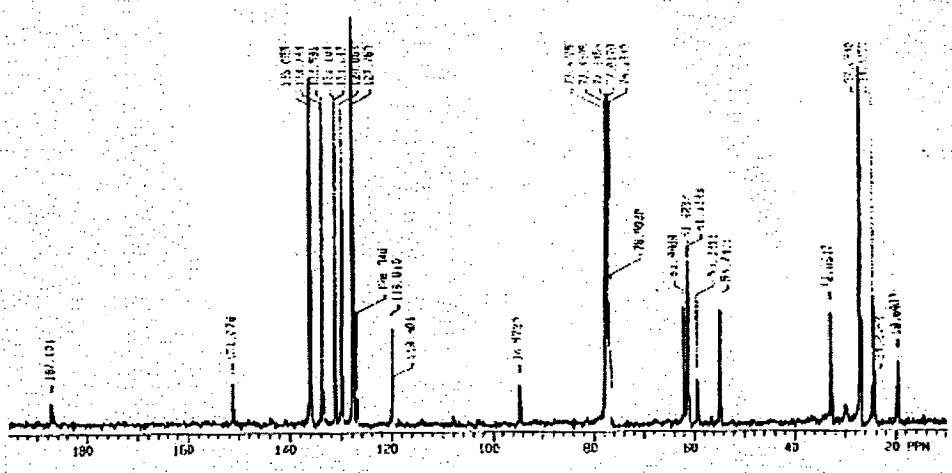

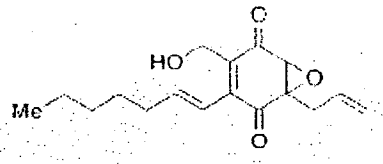

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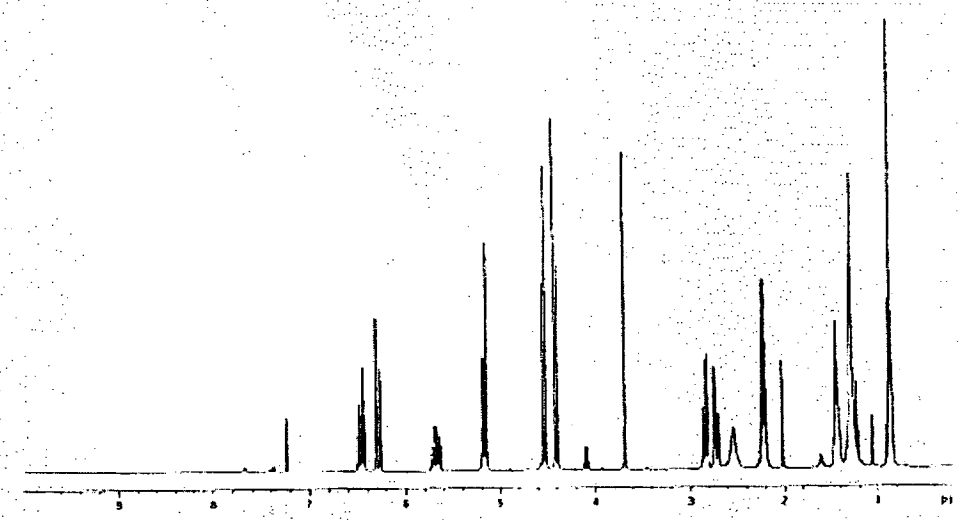

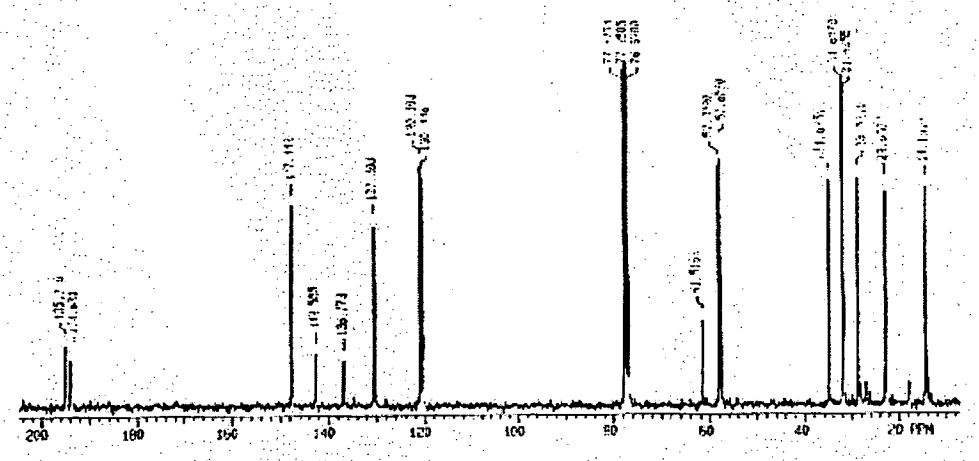

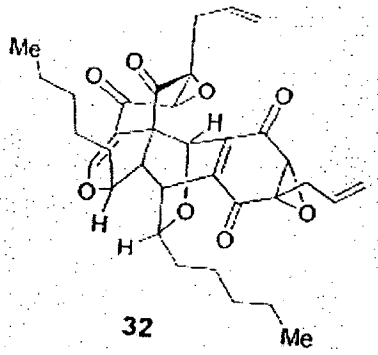

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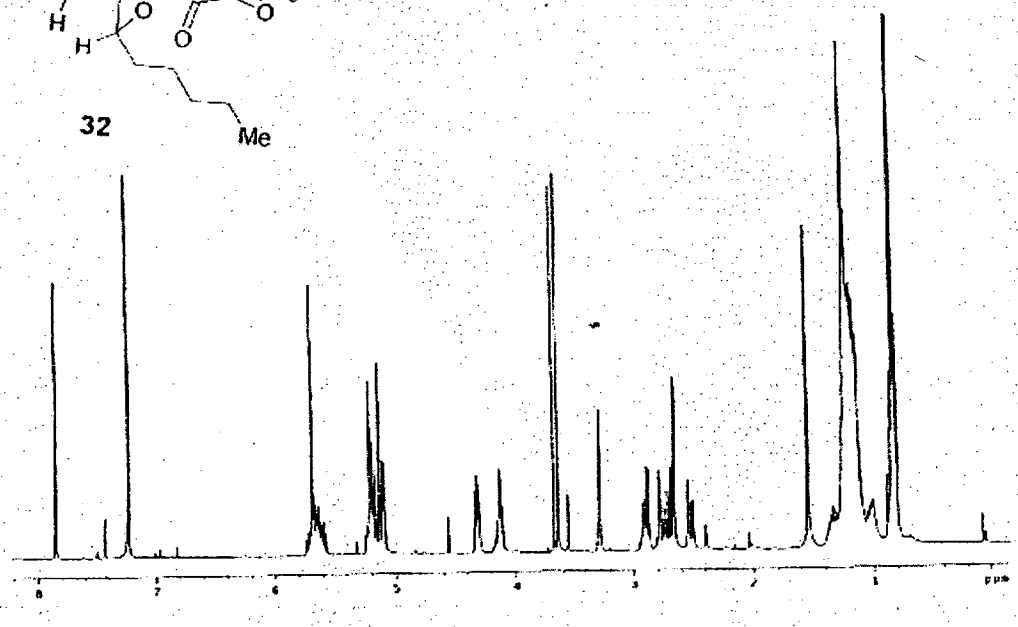

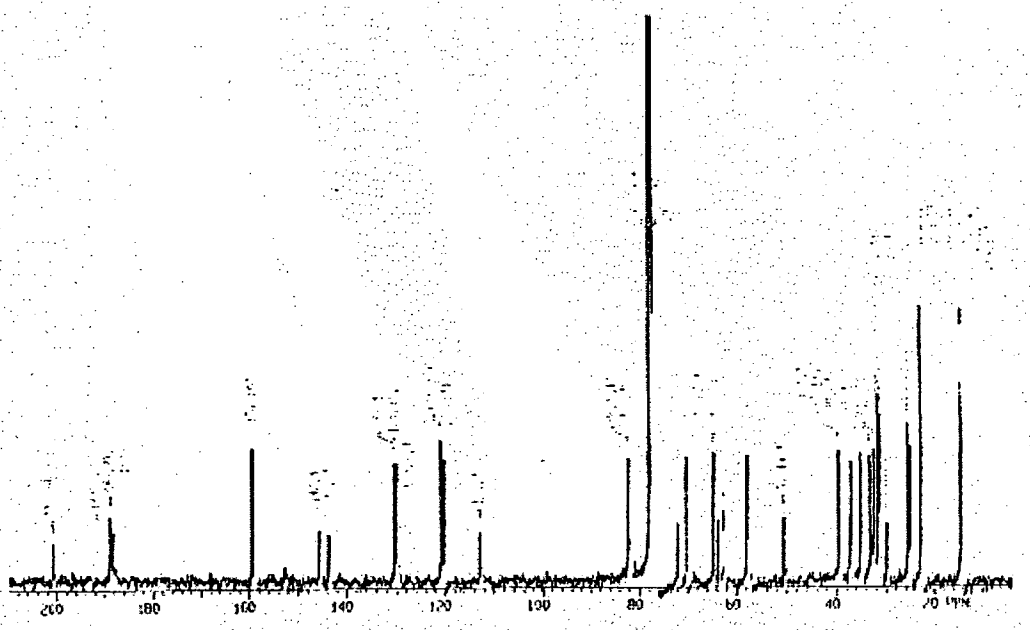

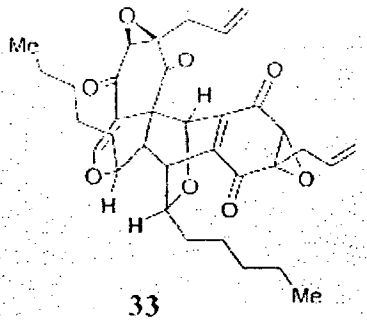

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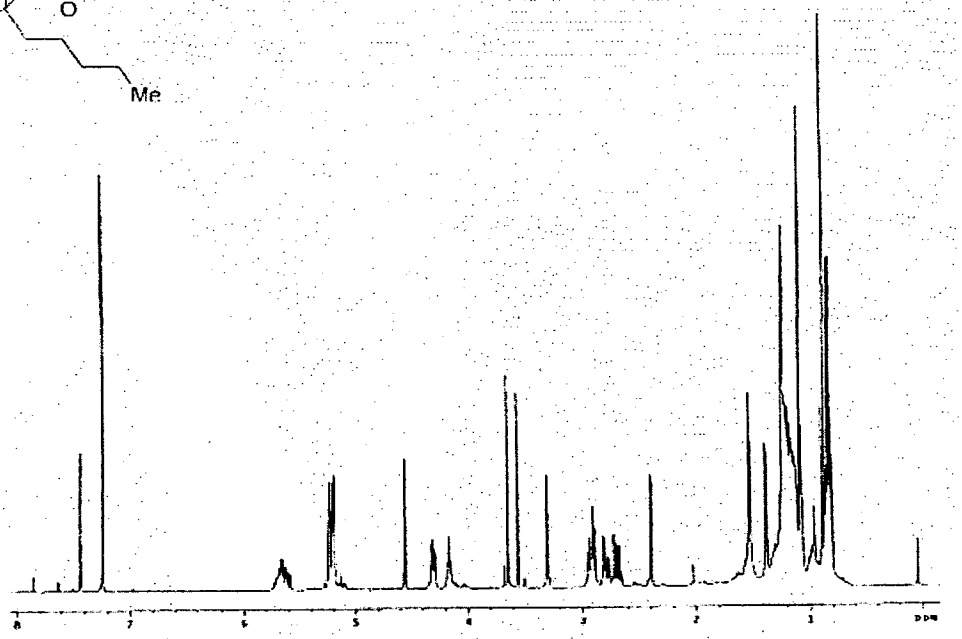

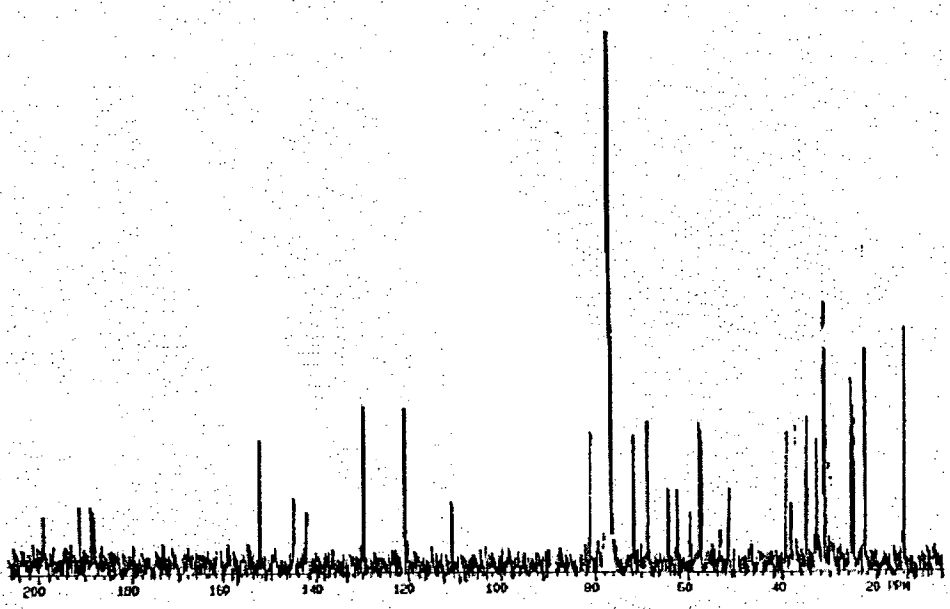

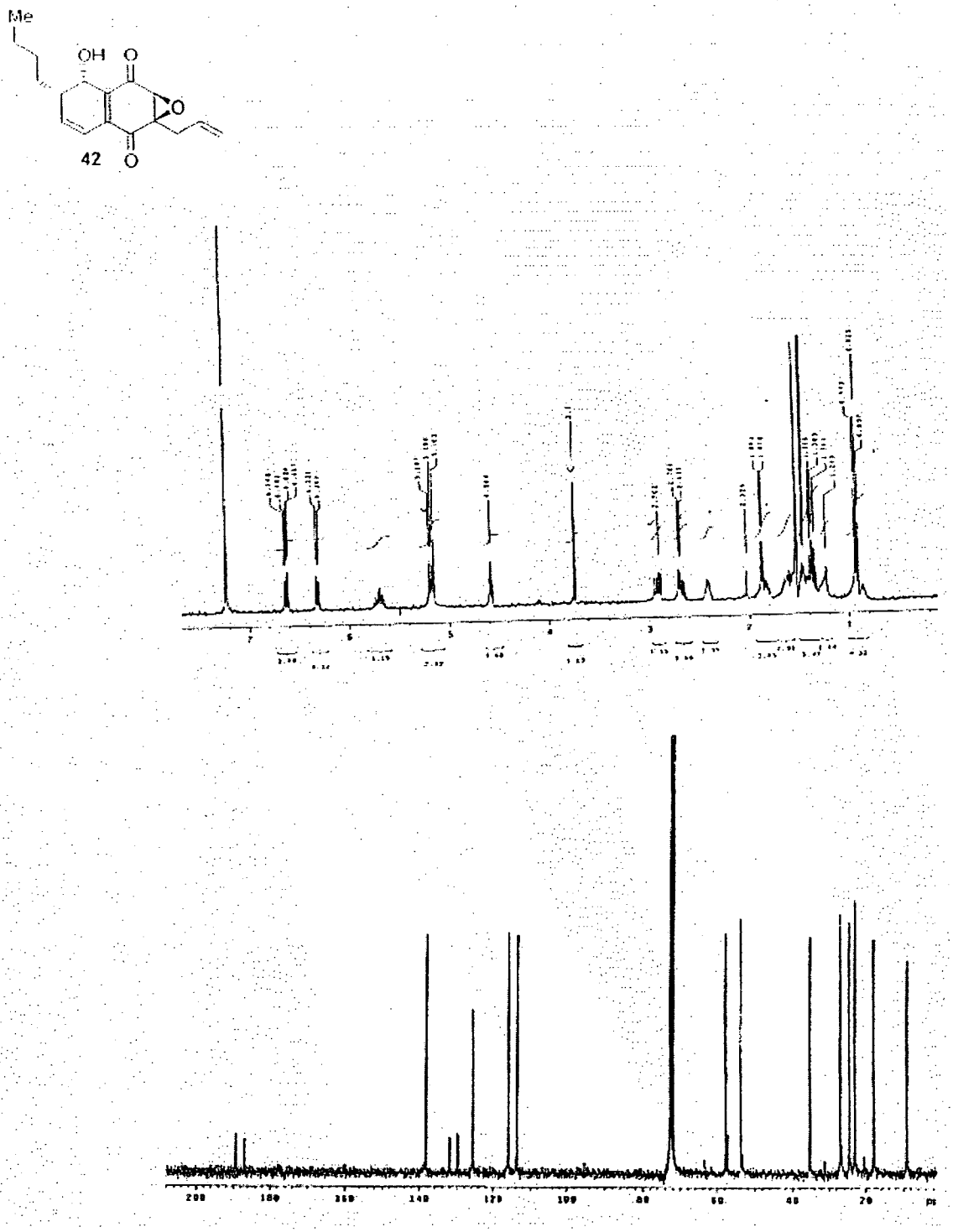
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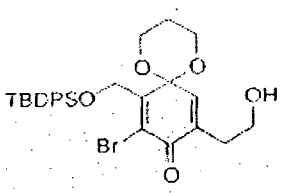

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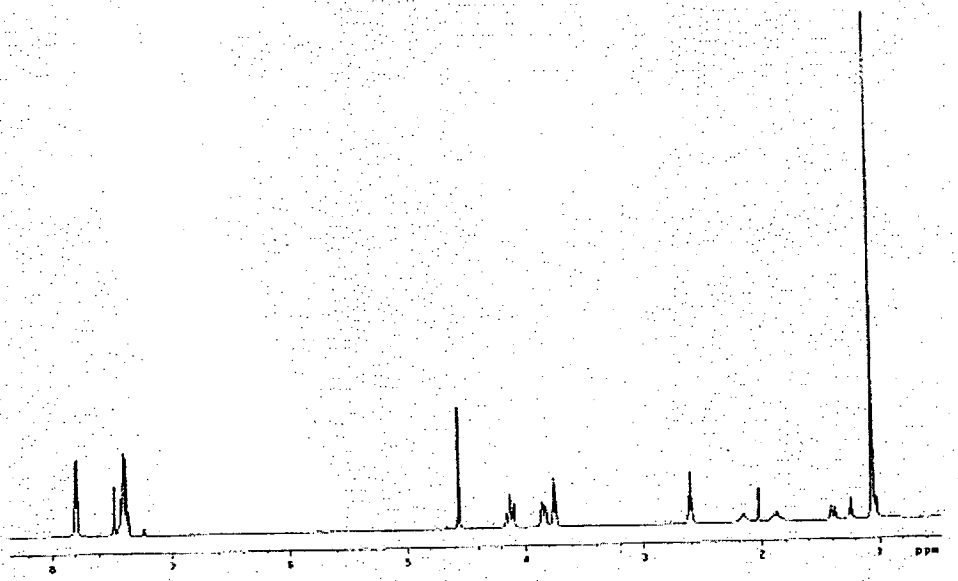

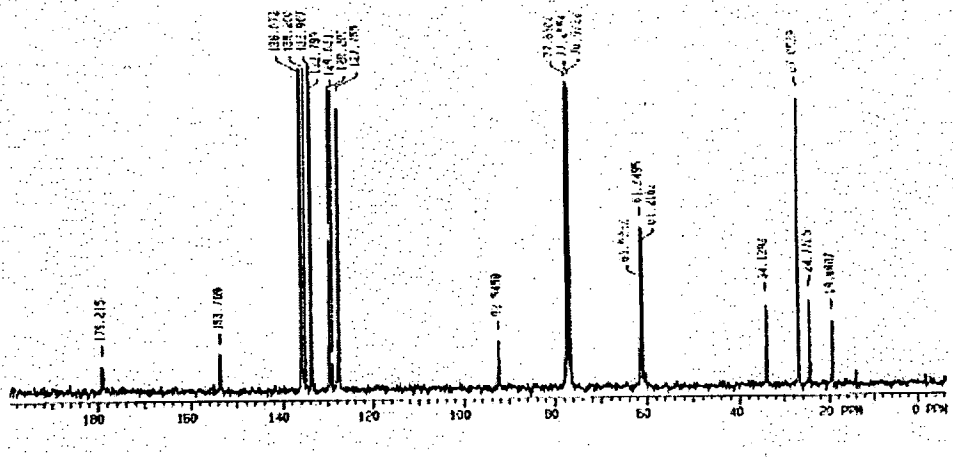

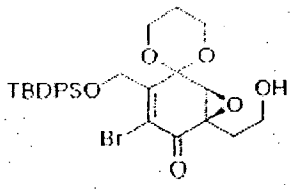

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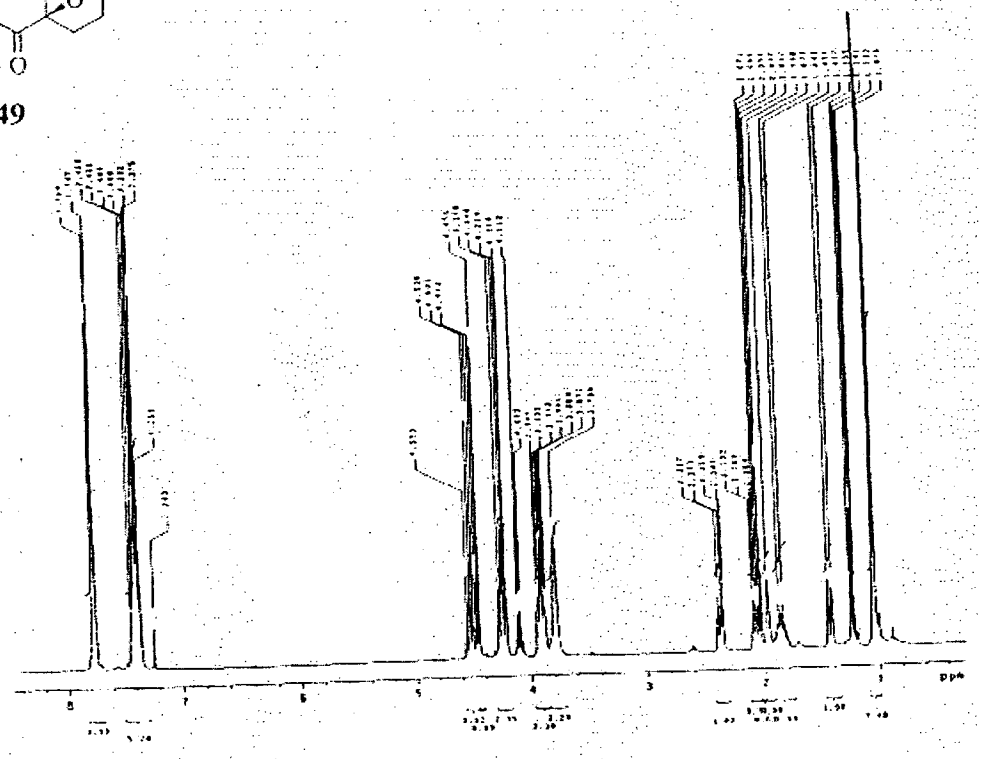

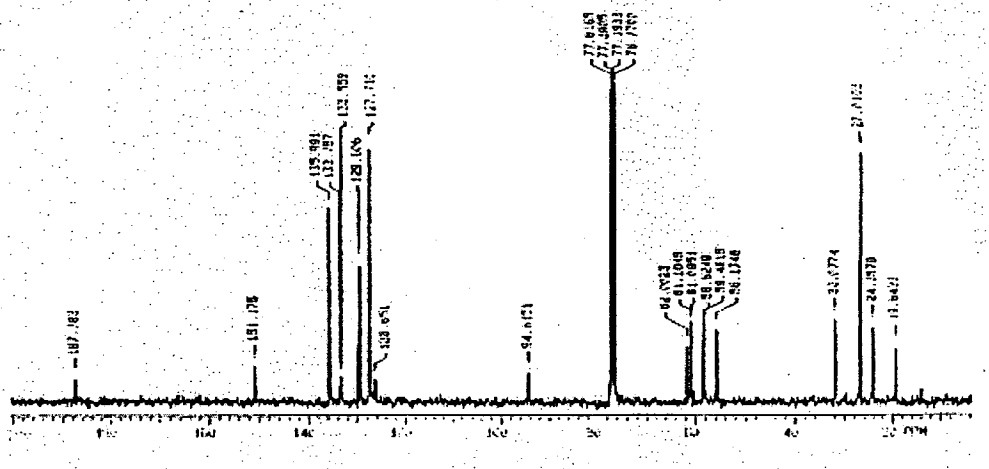

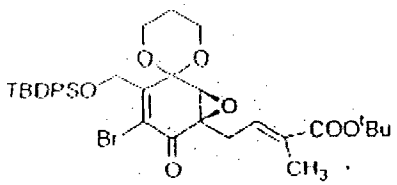

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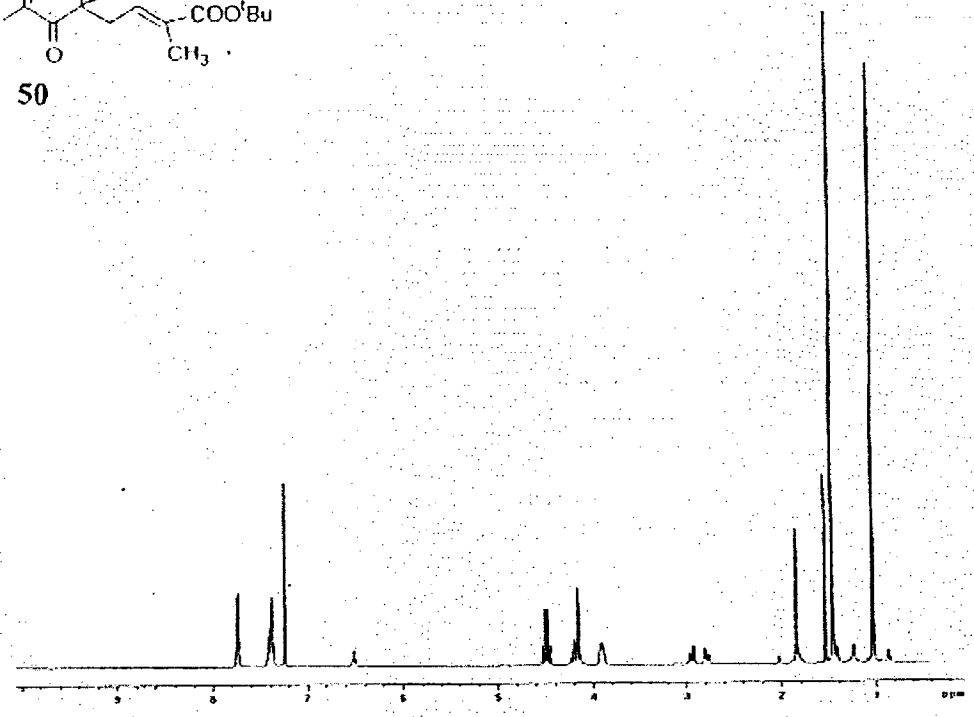

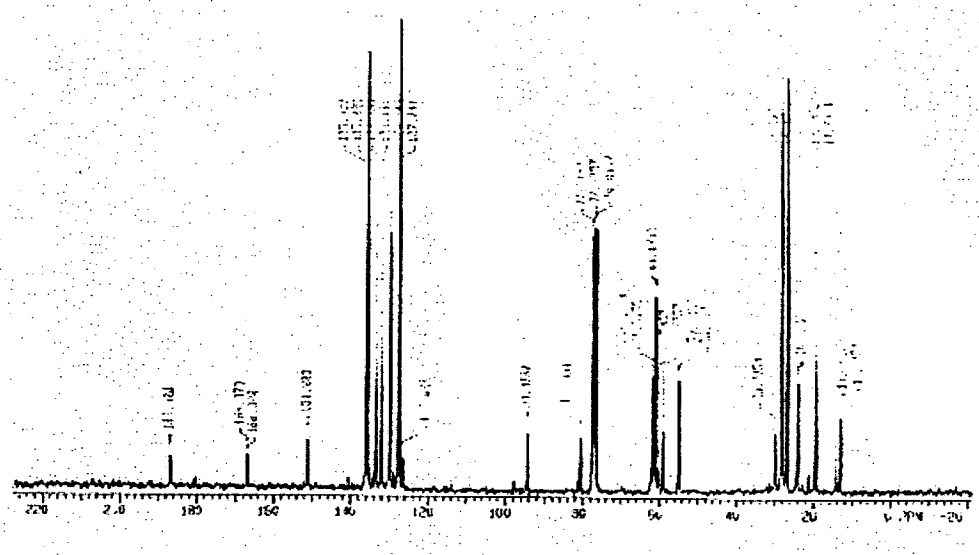

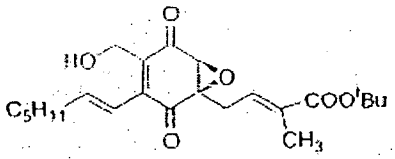

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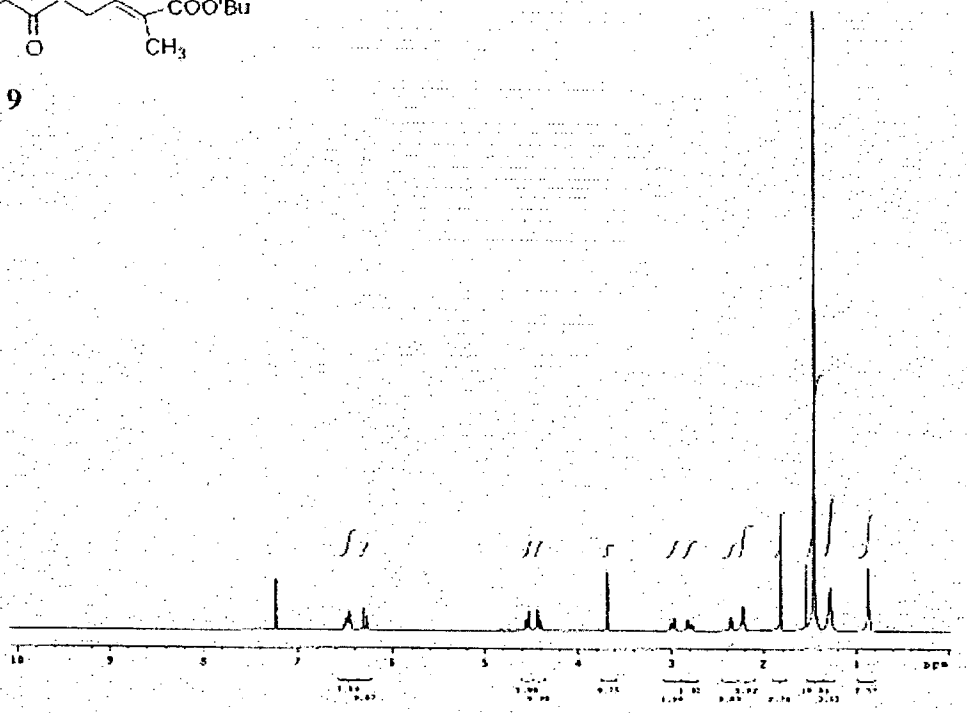

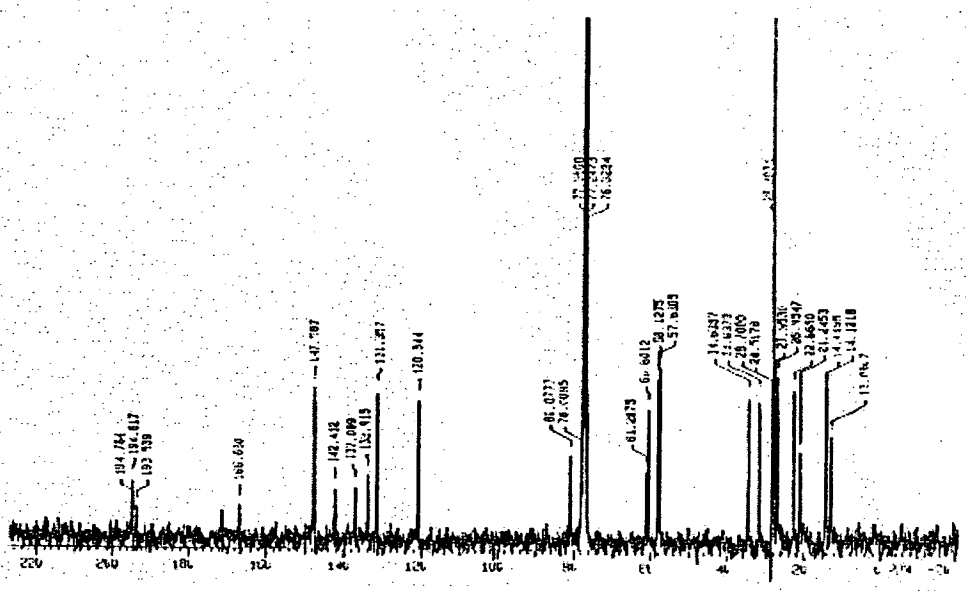

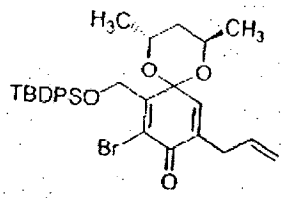

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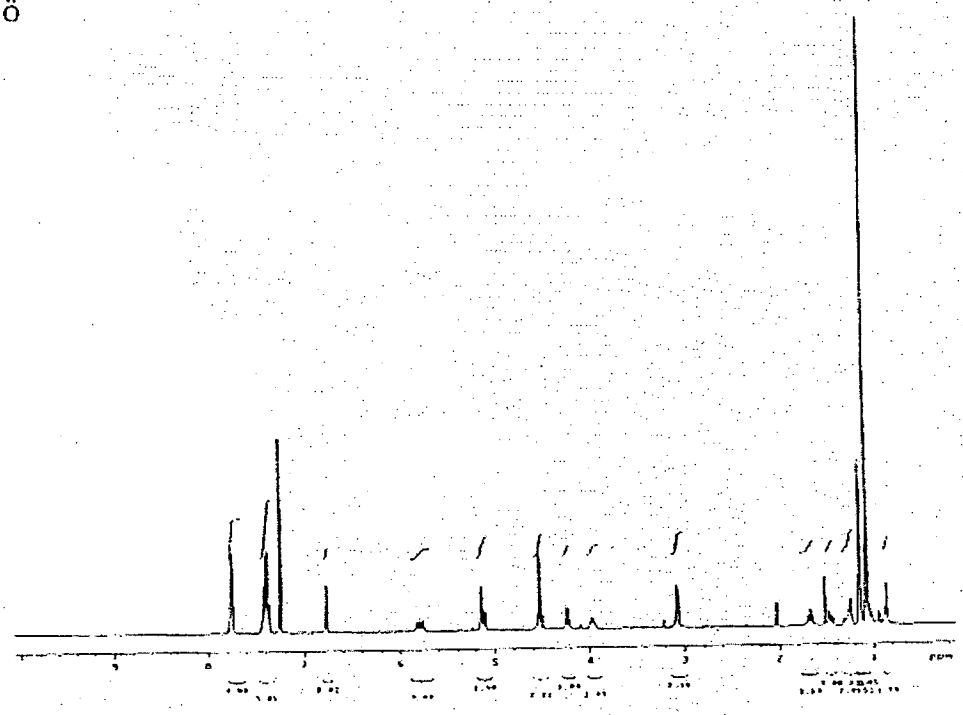

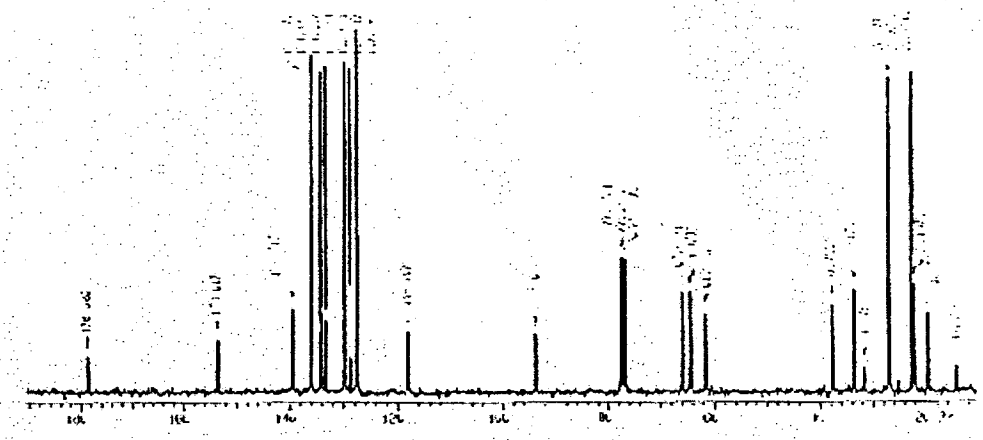

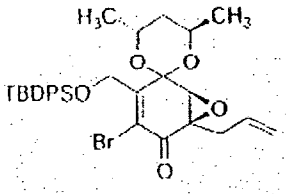

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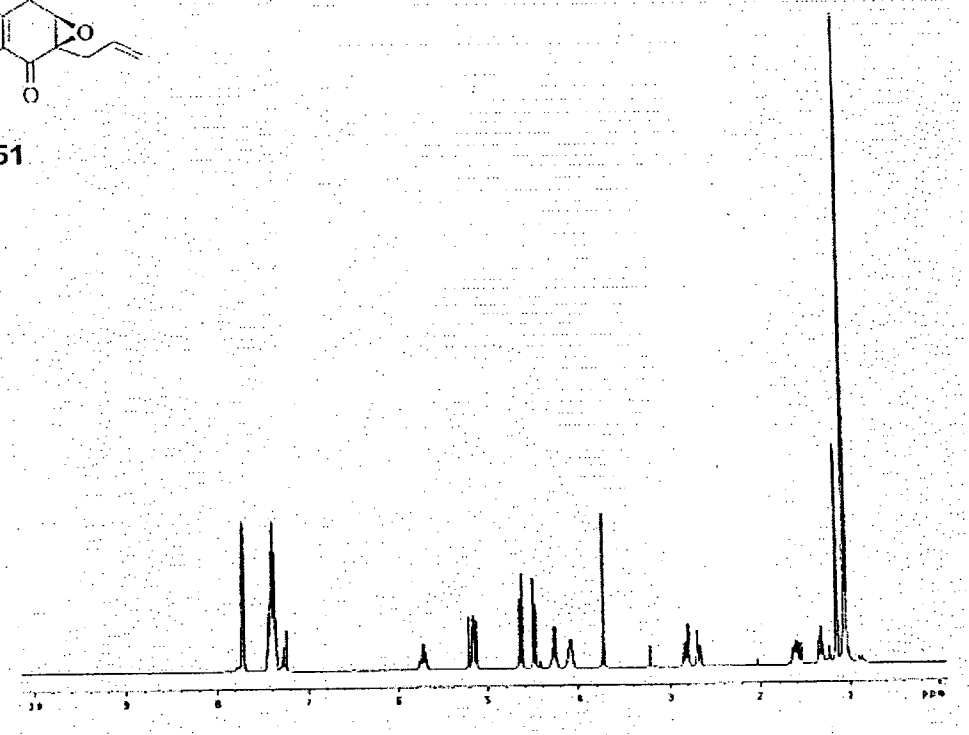

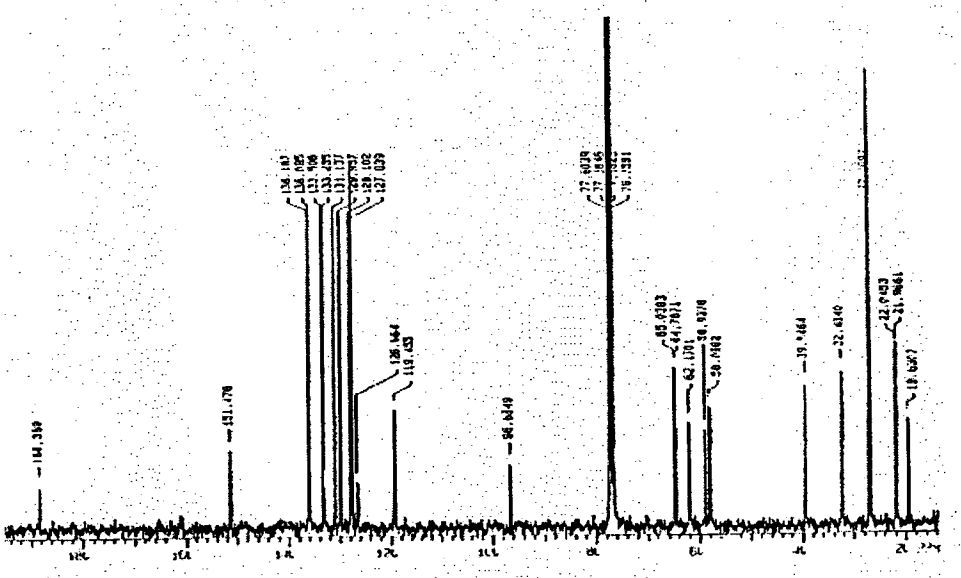

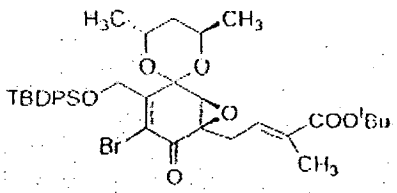

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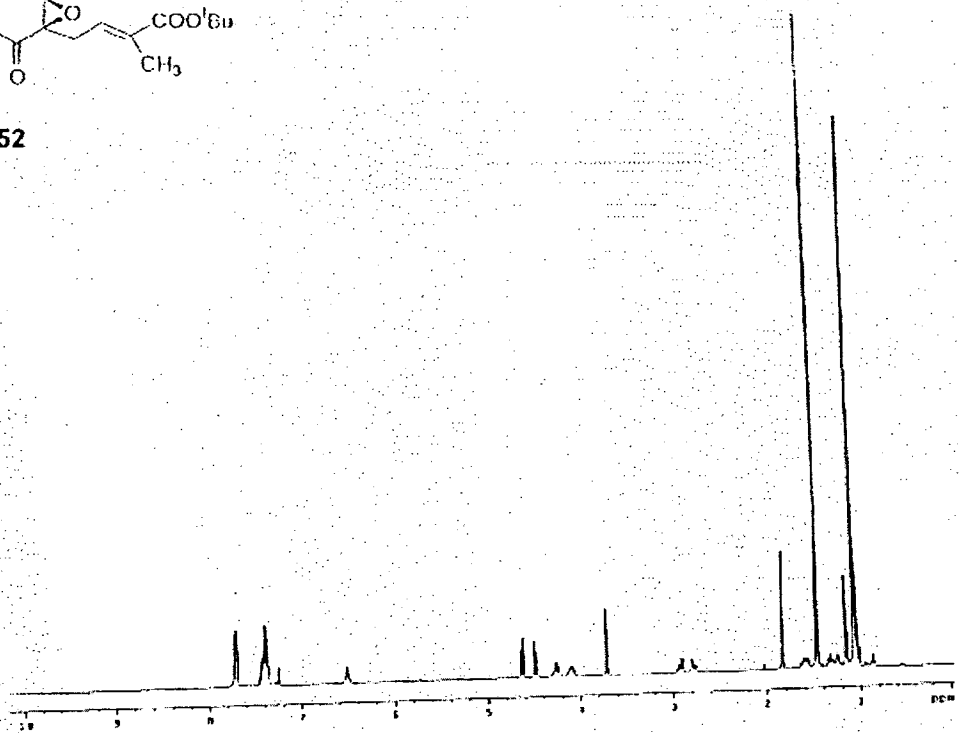
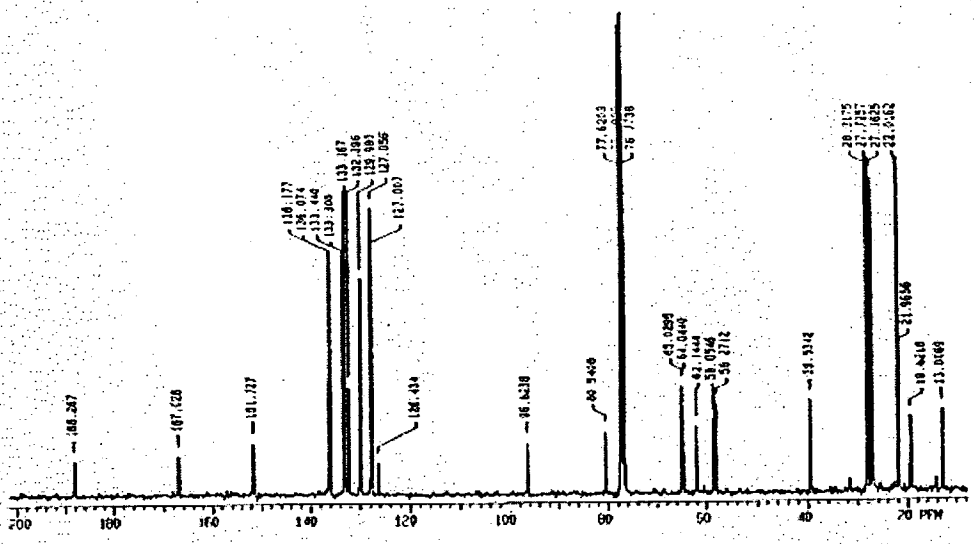
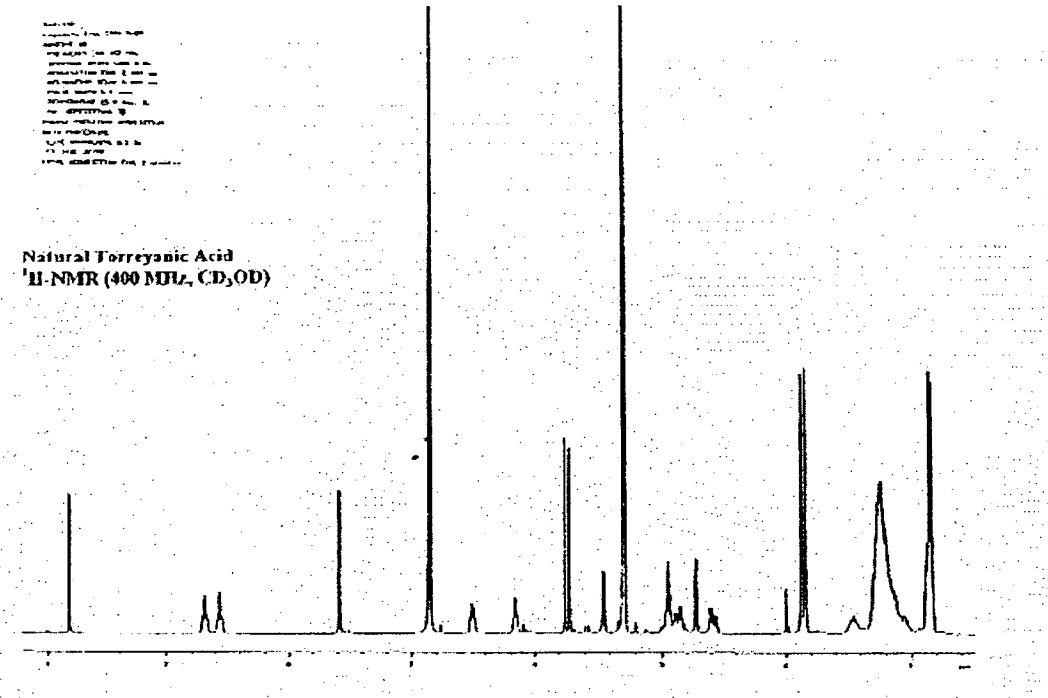
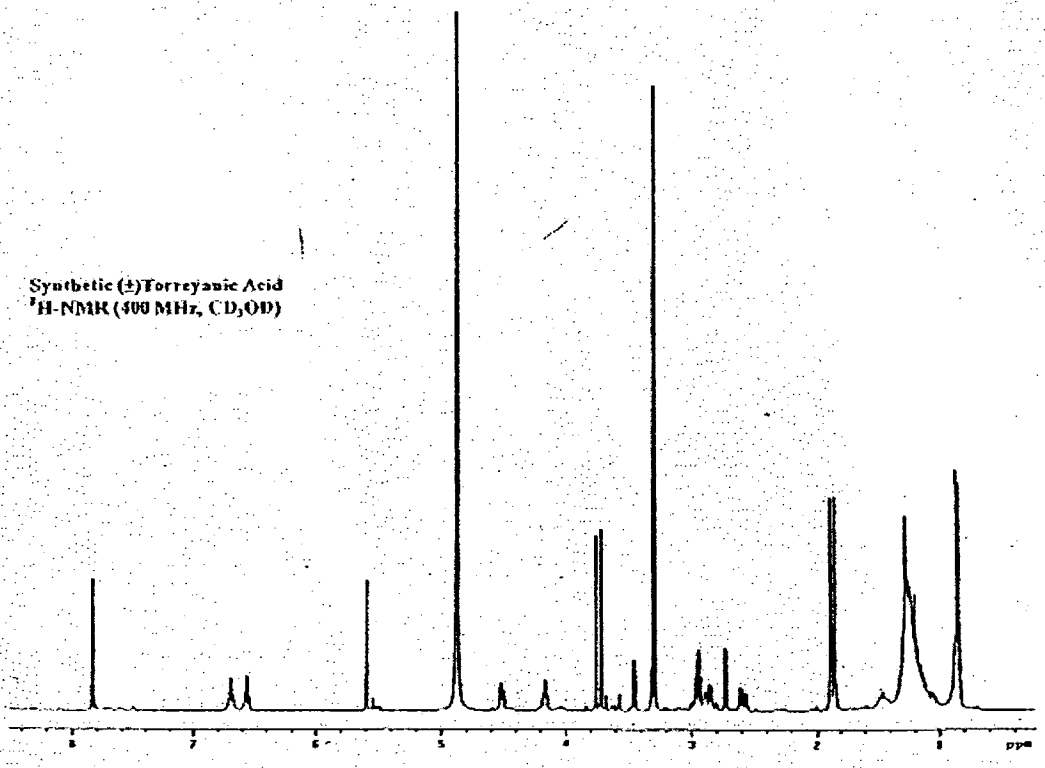
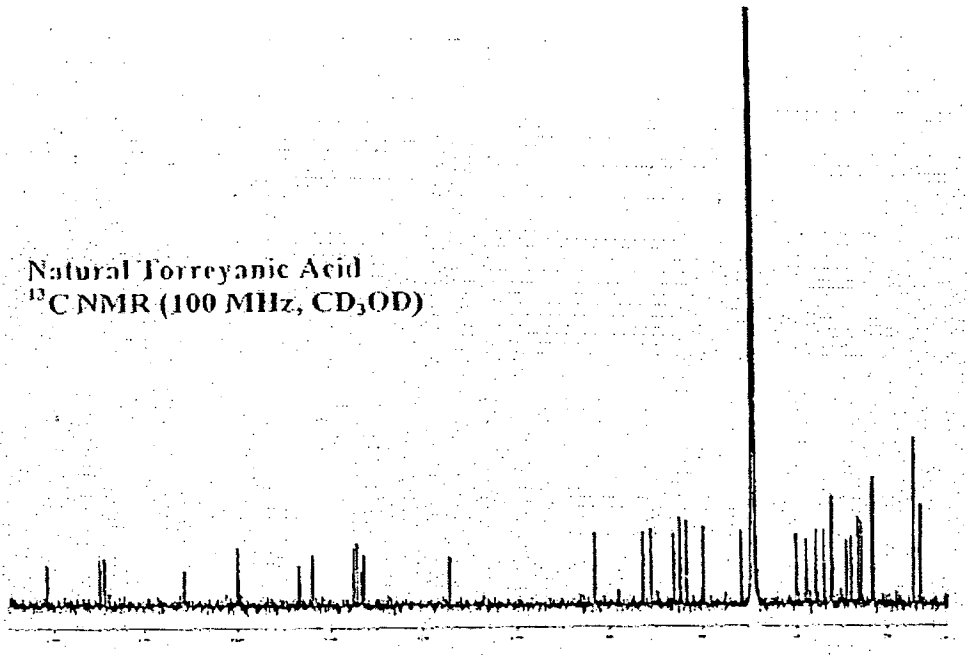
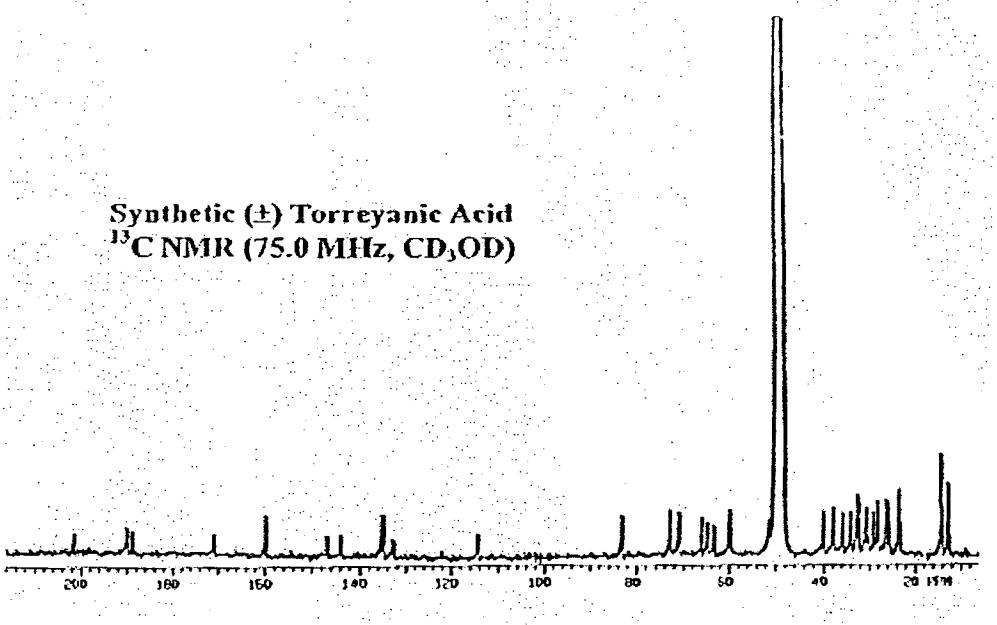


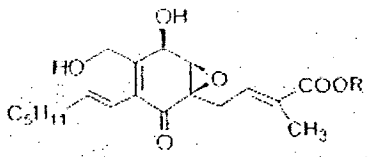



Natural Torreyanic Acid
¹H-NMR (400 MHz, CD₃OD)


Synthetic (±)Torreyanic Acid
¹H-NMR (400 MHz, CD₃OD)
ppm


Natural Torreyanic Acid
^{13}C NMR (100 MHz, CD_3OD)


Synthetic (±) Torreyanic Acid
^{13}C NMR (75.0 MHz, CD_3OD)
200
180
160
140
120
100
80
60
40



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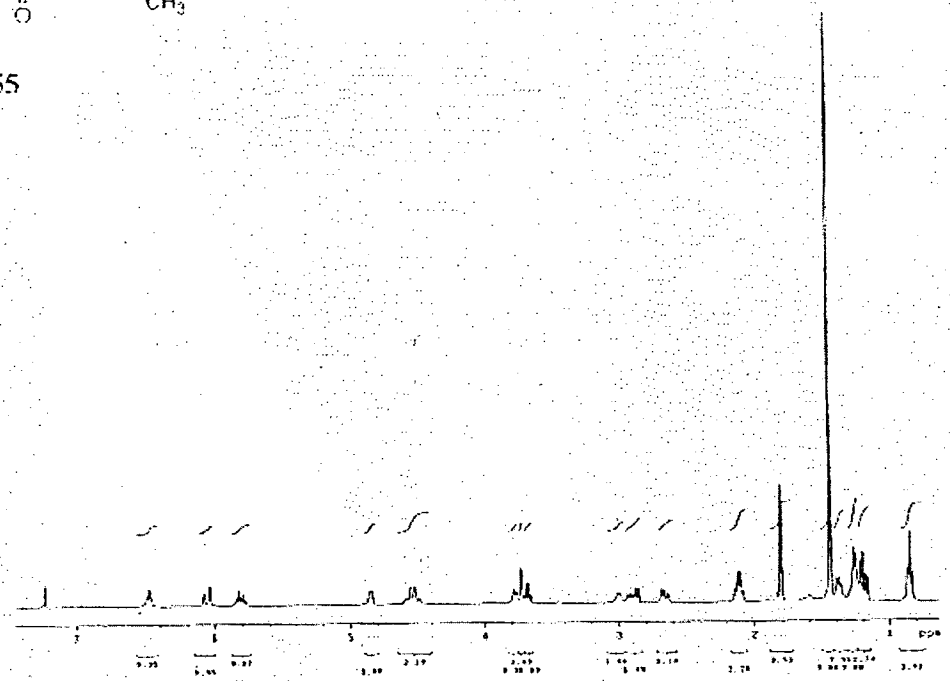

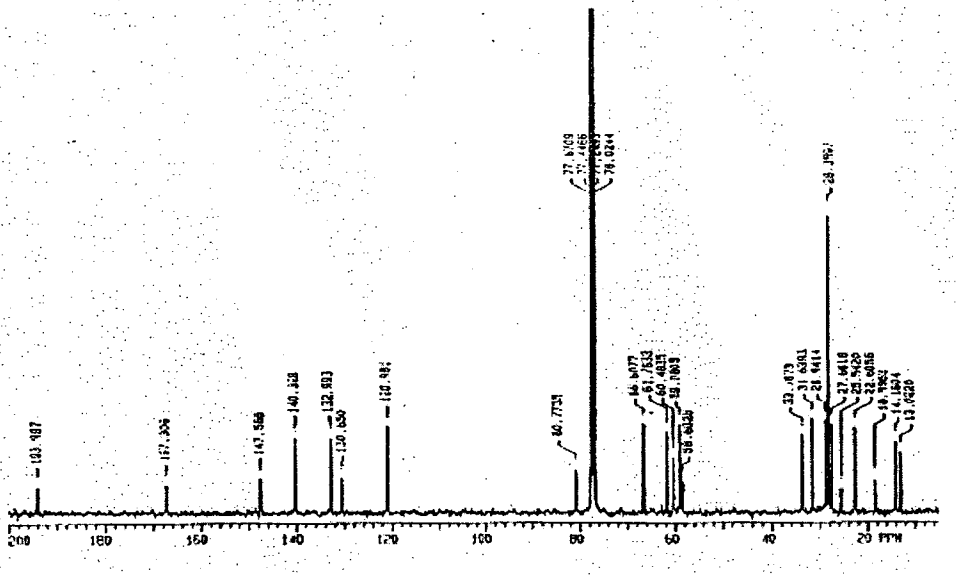

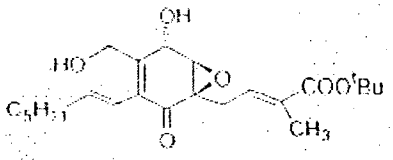

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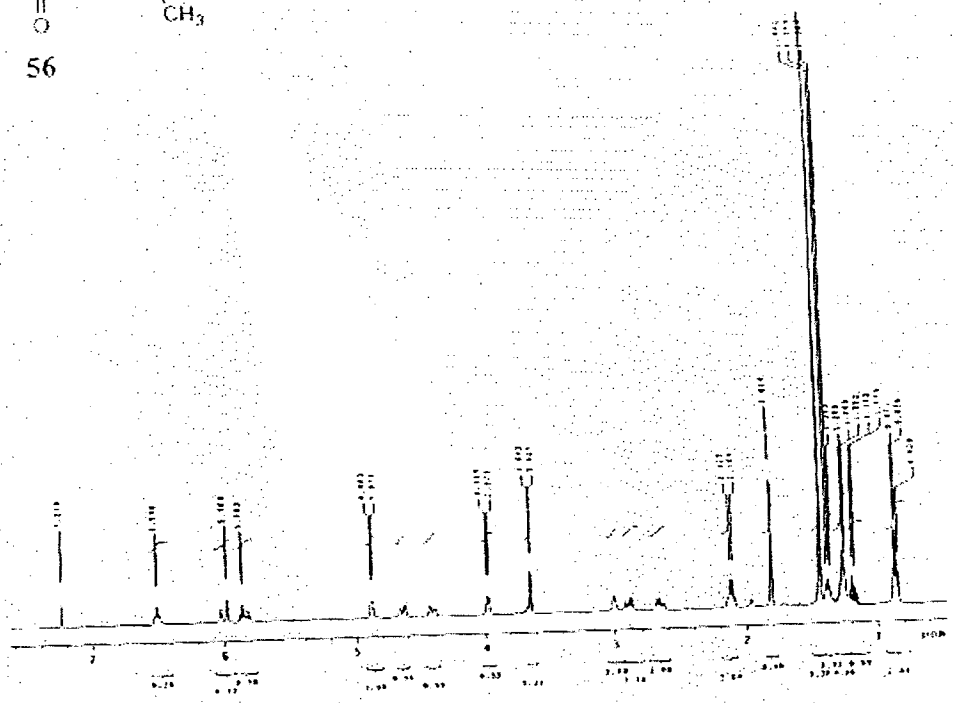

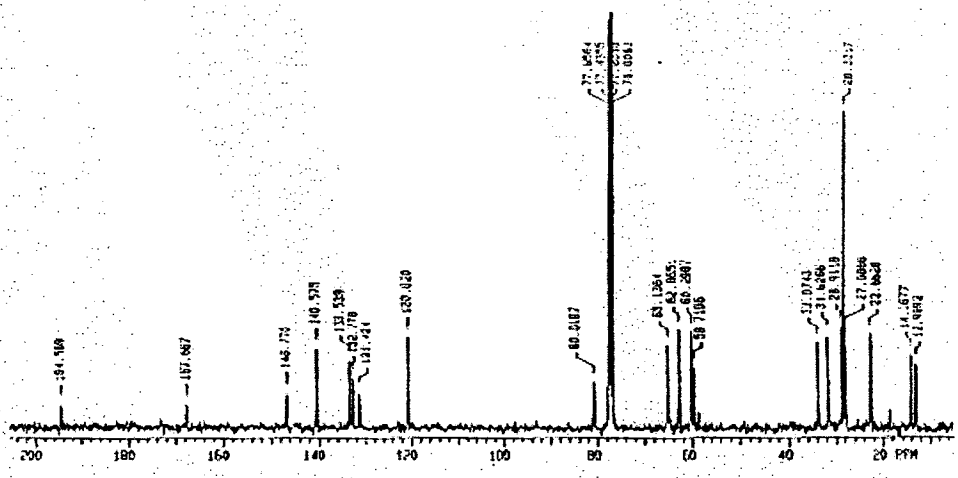

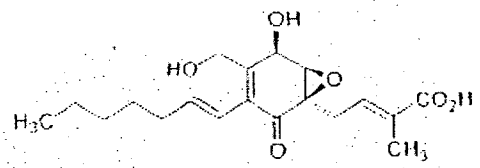

(2) *ambuic acid*