

Electronic Supplementary Information

Structure–activity studies of non-steroid analogues structurally-related to neuroprotective estrogens[†]

Mingxing Qian,^a Elizabeth B. Engler-Chiurazzi,^b Sara E. Lewis,^b Nigam P. Rath,^c

James W. Simpkins,^b and Douglas F. Covey^{*,a,d,e}

^a*Department of Developmental Biology, Campus Box 8103, Washington University in St. Louis, School of Medicine, 660 S. Euclid Ave., St. Louis, MO, 63110, USA. Email: dcovey@wustl.edu; Fax: +1 314 362 7058; Tele: +1 314-362 1726*

^b*Center for Basic and Translational Stroke Research, West Virginia University, Morgantown, WV 26506, USA*

^c*Department of Chemistry and Biochemistry and Center for Nanoscience, University of Missouri–St. Louis, St. Louis, MO, 63121, USA*

^d*Department of Anesthesiology, Washington University School of Medicine, St. Louis, MO, 63110, USA*

^e*Department of Psychiatry, Washington University School of Medicine, St. Louis MO, 63110.*

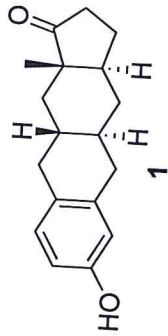
Copies of ¹H and ¹³C NMR spectra for compounds 1 to 26.

mq2153

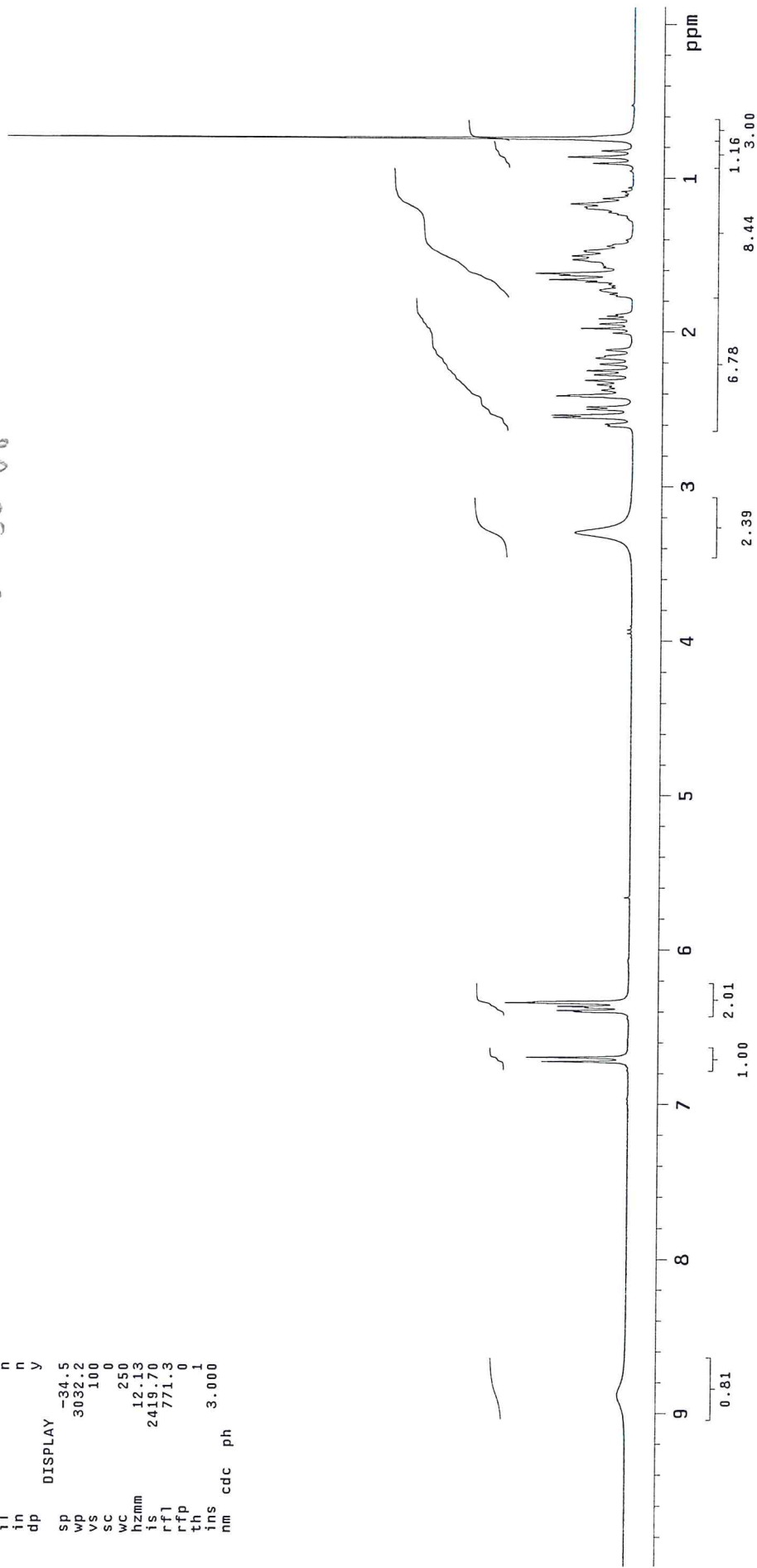
p01153 Sequence: s2pu1

exp1 std1h

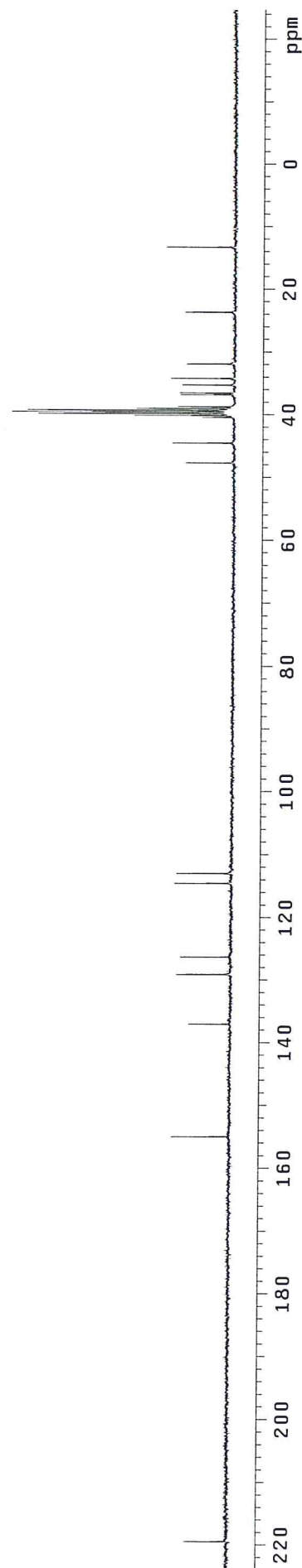
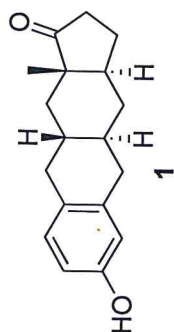
SAMPLE		DEC. & VT	
date	Jan 20 2010	dfrq	300.050
solvent	DMSO	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	300.050	dmm	nnn
tn	1.998	dmf	c
at	17984	wtfile	200
np	4500.5	proc	ft
sw	2600	fn	not used
bs	16		
tpwr	49		
pw	7.0	werr	
di	1.000	wexp	
tof	0	wbs	
nt	8	wnt	
ct	8		
alock	n		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-34.5		
wp	3032.2		
vs	100		
sc	0		
wc	250		
hzmm	12.13		
is	2419.70		
rfl	771.3		
rfp	0		
th	1		
ins	3.000		
nm	cdc	ph	



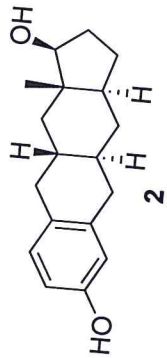
in DMSO-d6



INDEX	FREQUENCY	PPM	HEIGHT
1	16559.501	219.484	6.8
2	11692.423	154.975	9.3
3	10338.803	137.033	6.7
4	9739.866	129.095	8.7
5	9528.005	126.287	8.1
6	8640.479	114.523	9.1
7	8522.524	112.960	8.8
8	3595.896	47.661	7.7
9	3356.550	44.489	9.8
10	3045.057	40.360	5.1
11	3024.444	40.087	15.9
12	3003.830	39.814	31.2
13	2982.072	39.525	35.4
14	2961.458	39.252	32.9
15	2940.845	38.979	15.6
16	2916.795	38.660	9.0
17	2772.501	36.747	8.5
18	2751.887	36.474	8.7
19	2655.691	35.199	8.3
20	2575.527	34.137	10.1
21	2402.603	31.845	7.6
22	1783.053	23.633	7.9
23	997.449	13.220	10.9

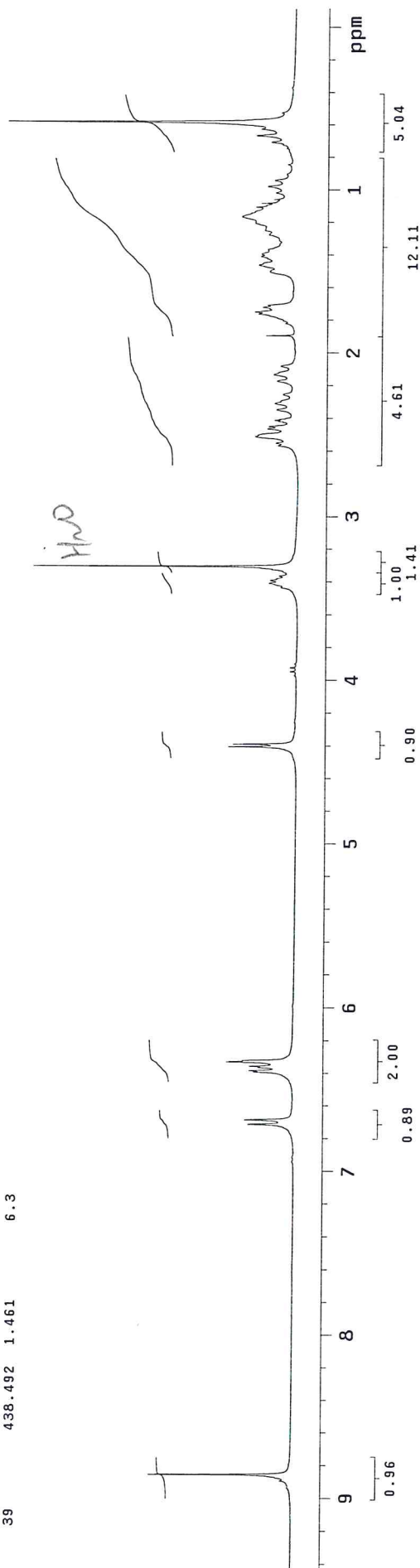


2155

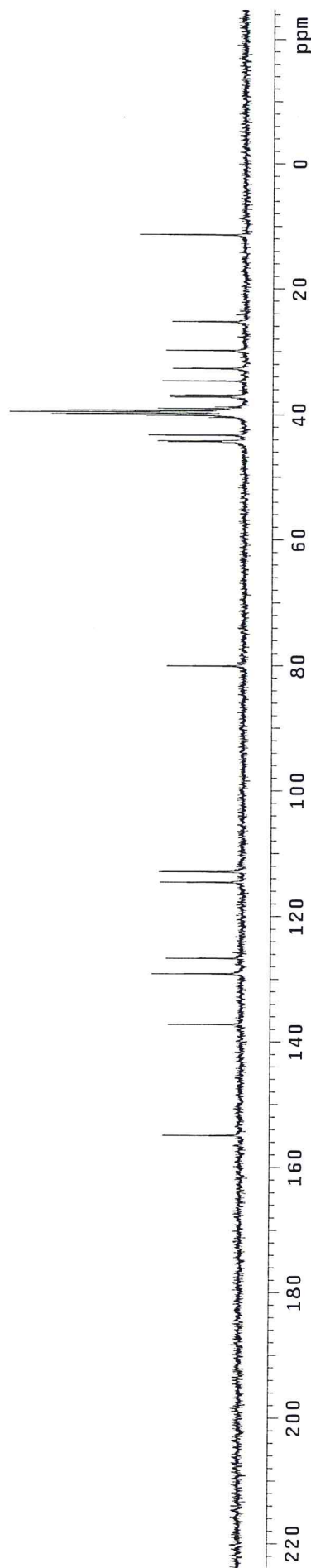
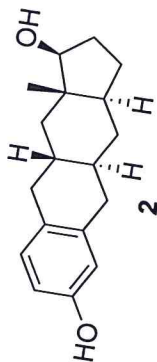


in DMSO-d6

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2668.801	8.895	1.8	40	422.285	1.407	6.0
2	2657.539	8.857	22.8	41	418.164	1.394	6.0
3	2014.185	6.713	7.3	42	409.923	1.366	4.9
4	2005.944	6.685	7.8	43	382.178	1.274	4.8
5	1917.765	6.392	6.5	44	374.212	1.247	5.4
6	1915.293	6.383	7.1	45	349.489	1.165	9.1
7	1909.524	6.364	5.7	46	331.358	1.104	6.9
8	1907.326	6.357	7.1	47	324.216	1.081	6.0
9	1899.085	6.329	10.8	48	317.074	1.057	4.0
10	1321.386	4.404	10.8	49	305.262	1.017	3.7
11	1316.441	4.387	10.1	50	293.449	0.978	5.0
12	1029.927	3.433	2.6	51	282.461	0.941	3.9
13	1022.235	3.407	4.5	52	270.924	0.903	2.0
14	1016.741	3.389	4.2	53	253.068	0.843	1.8
15	1017.290	3.390	4.2	54	223.126	0.744	2.1
16	1008.774	3.362	2.8	55	211.588	0.705	4.5
17	991.194	3.303	42.1	56	199.226	0.664	6.9
18	769.509	2.565	3.2	57	187.139	0.624	6.1
19	765.113	2.550	3.5	58	174.228	0.581	46.4
20	753.027	2.510	6.8	59	157.197	0.524	2.9
21	738.742	2.462	4.9	60	110.772	0.369	1.2
22	734.896	2.449	4.6				
23	725.007	2.416	3.2				
24	723.359	2.411	3.7				
25	721.436	2.404	2.9				
26	704.404	2.348	3.4				
27	692.592	2.308	3.7				
28	676.110	2.253	2.4				
29	651.661	2.172	3.3				
30	639.849	2.132	3.9				
31	624.191	2.080	2.8				
32	567.877	1.893	5.2				
33	545.626	1.818	2.1				
34	528.045	1.760	6.4				
35	524.474	1.748	6.9				
36	516.233	1.720	5.7				
37	512.387	1.708	4.9				
38	450.030	1.500	4.6				
39	438.492	1.461	6.3				

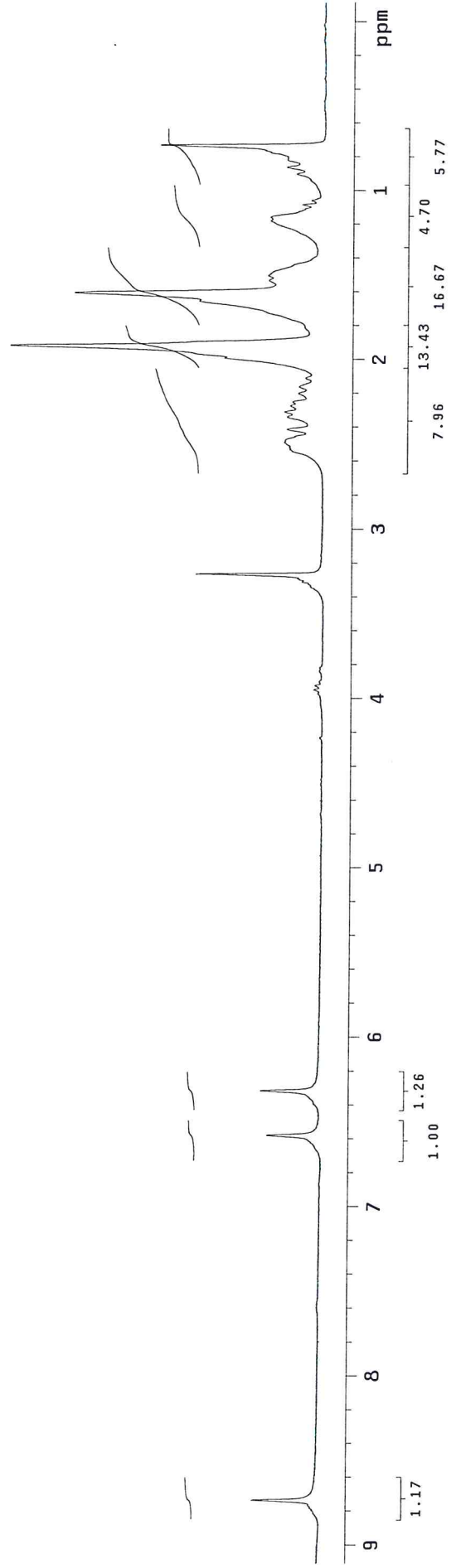
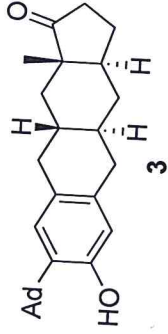


INDEX	FREQUENCY	PPM	HEIGHT
1	11686.697	154.899	12.4
2	10350.255	137.185	11.7
3	9738.721	129.080	14.3
4	9552.054	126.605	12.0
5	8641.624	114.538	13.1
6	8515.853	112.869	13.2
7	6034.016	79.976	12.1
8	3339.372	44.261	12.2
9	3326.775	44.094	13.8
10	3259.209	43.198	15.2
11	3043.912	40.345	5.7
12	3022.153	40.056	15.6
13	3001.540	39.783	30.7
14	2980.926	39.510	37.4
15	2974.055	39.419	17.6
16	2960.313	39.237	28.2
17	2938.554	38.948	13.8
18	2917.941	38.675	4.7
19	2797.695	37.081	11.8
20	2777.082	36.808	11.9
21	2606.448	34.547	13.1
22	2456.427	32.558	11.5
23	2242.276	29.720	12.5
24	1897.572	25.151	11.5
25	849.719	11.262	16.8

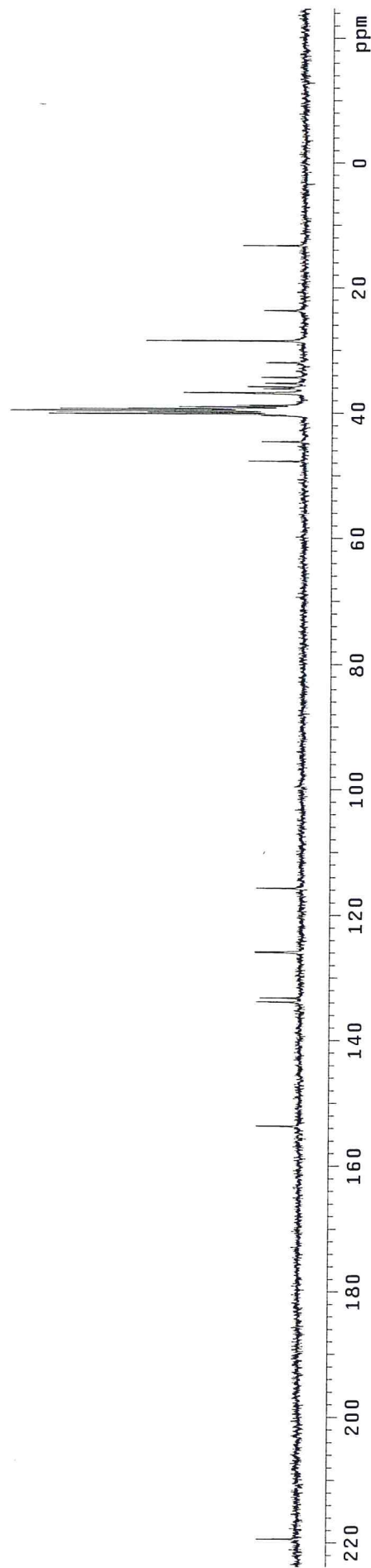
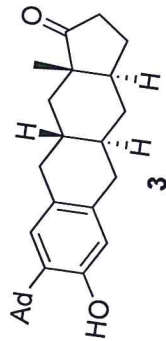


MQ2156

INDEX	FREQUENCY	PPM	HEIGHT
1	2622.377	8.740	10.5
2	1974.903	6.582	8.4
3	1895.514	6.317	9.5
4	979.656	3.265	20.3
5	746.983	2.490	6.3
6	723.633	2.412	5.9
7	701.657	2.338	5.8
8	692.317	2.307	6.3
9	682.153	2.273	5.4
10	659.353	2.197	4.1
11	647.815	2.159	4.0
12	632.432	2.108	3.0
13	576.942	1.923	50.0
14	482.719	1.609	39.8
15	460.194	1.534	8.9
16	451.129	1.504	9.0
17	353.609	1.179	8.7
18	347.840	1.159	8.7
19	324.765	1.082	3.7
20	317.623	1.059	2.2
21	270.374	0.901	4.6
22	258.287	0.861	6.1
23	220.104	0.734	26.3

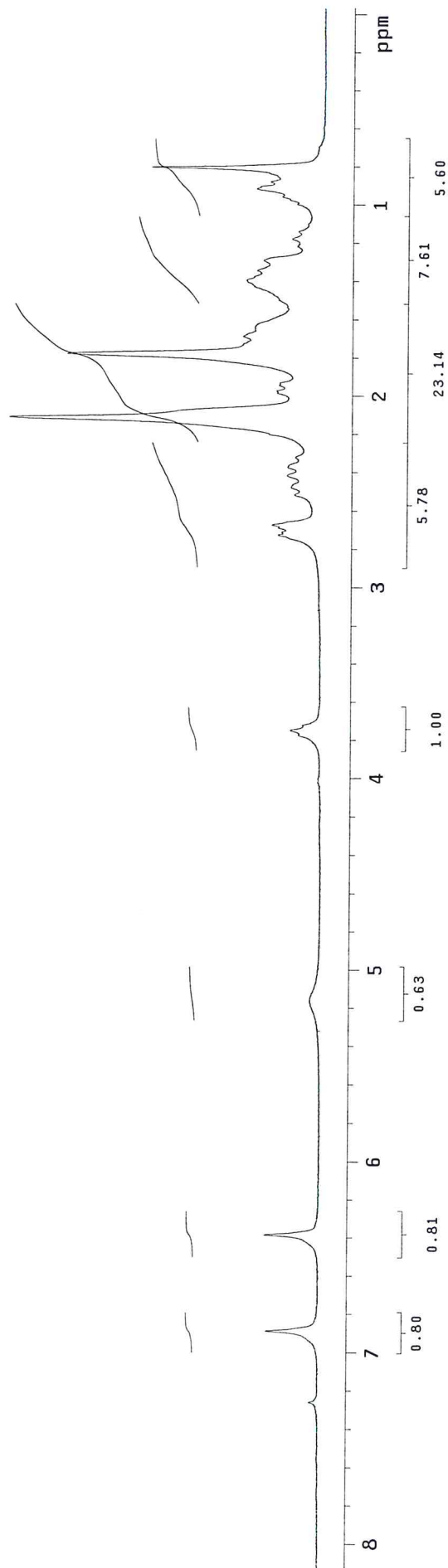
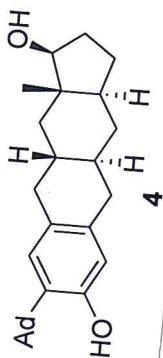


INDEX	FREQUENCY	PPM	HEIGHT
1	16552.630	219.393	6.5
2	11589.356	153.608	6.9
3	10094.876	133.800	7.0
4	10045.633	133.148	6.4
5	9497.085	125.877	7.3
6	9487.923	125.755	7.3
7	8724.078	115.631	7.1
8	3592.460	47.615	8.7
9	3356.550	44.489	6.6
10	3043.912	40.345	6.8
11	3022.153	40.056	40.5
12	3001.540	39.783	39.4
13	2980.926	39.510	46.8
14	2959.168	39.222	38.8
15	2938.554	38.948	19.8
16	2917.941	38.675	10.6
17	2766.775	36.672	19.1
18	2718.677	36.034	6.4
19	2694.628	35.715	8.9
20	2652.256	35.154	6.1
21	2581.253	34.213	6.7
22	2406.039	31.890	6.0
23	2143.789	28.414	25.1
24	1780.762	23.603	6.3
25	994.014	13.175	9.7

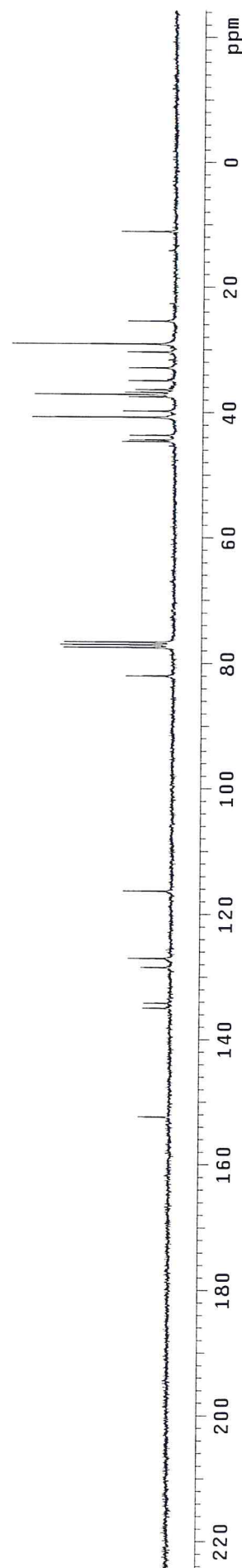
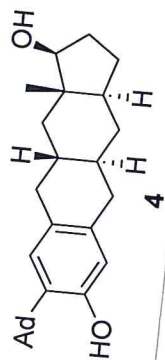


MQ2157

INDEX	FREQUENCY	PPM	HEIGHT
1	2067.090	6.889	8.3
2	1915.729	6.385	8.6
3	1551.748	5.172	1.7
4	1124.586	3.748	5.1
5	817.469	2.724	7.1
6	801.811	2.672	8.2
7	754.013	2.513	4.6
8	742.200	2.474	5.2
9	724.619	2.415	5.8
10	710.610	2.368	5.7
11	696.050	2.320	4.5
12	634.517	2.115	50.0
13	591.389	1.971	7.5
14	582.324	1.941	7.1
15	534.251	1.781	40.8
16	505.956	1.686	12.9
17	417.777	1.392	12.5
18	402.943	1.343	10.7
19	387.285	1.291	9.7
20	353.222	1.177	5.2
21	341.410	1.138	4.2
22	274.107	0.914	10.9
23	263.119	0.877	8.7
24	240.868	0.803	27.7

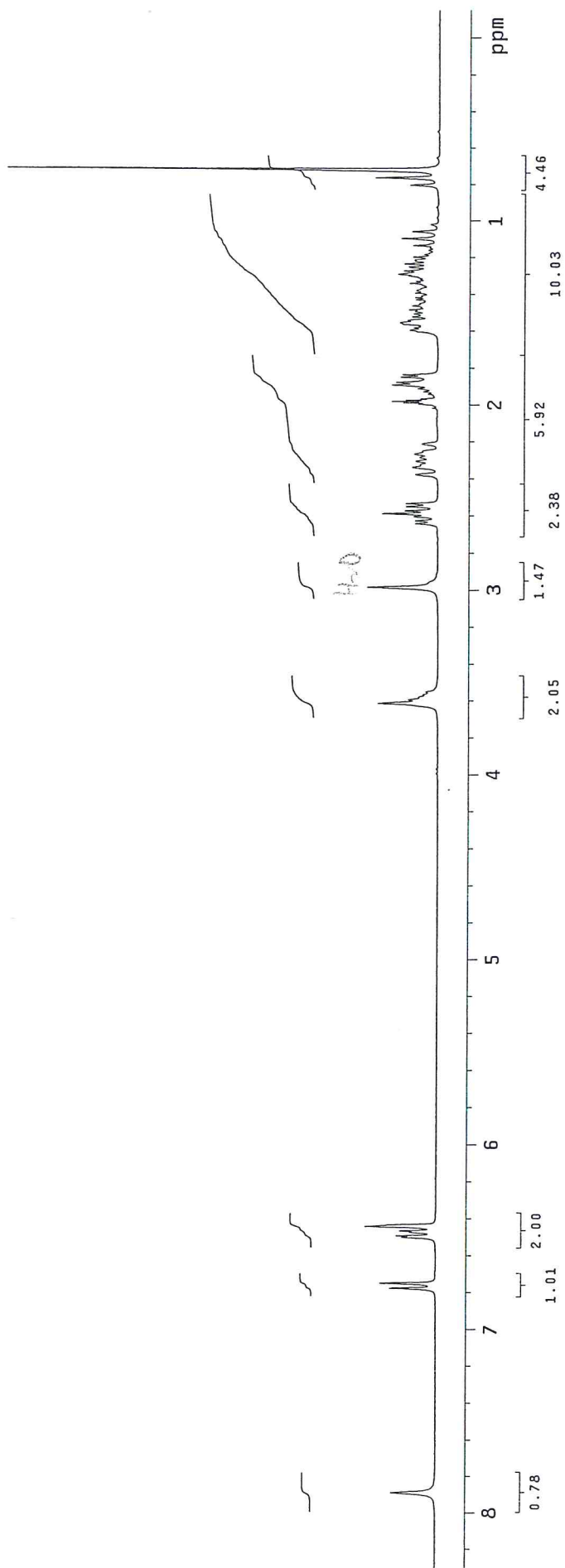
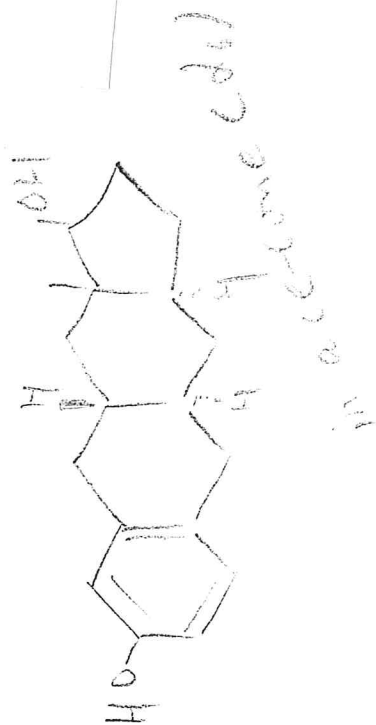
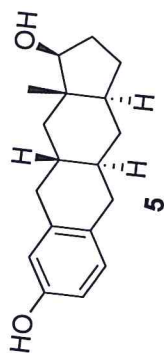


INDEX	FREQUENCY	PPM	HEIGHT
1	11494.166	152.348	5.0
2	10180.628	134.937	4.4
3	10118.787	134.118	4.3
4	9688.194	128.411	4.7
5	9580.546	126.984	6.8
6	8772.038	116.268	7.7
7	6179.317	81.903	7.5
8	5841.485	77.425	17.4
9	5809.419	77.000	18.0
10	5777.354	76.575	17.3
11	3363.283	44.578	8.3
12	3341.524	44.290	7.2
13	3286.555	43.561	7.1
14	3070.113	40.692	22.7
15	2995.676	39.706	8.2
16	2825.042	37.444	7.3
17	2796.412	37.065	22.3
18	2768.927	36.700	7.9
19	2738.007	36.290	6.2
20	2630.358	34.864	7.4
21	2475.757	32.815	7.3
22	2286.800	30.310	7.5
23	2190.604	29.035	26.0
24	1914.612	25.377	7.5
25	832.403	11.033	8.6



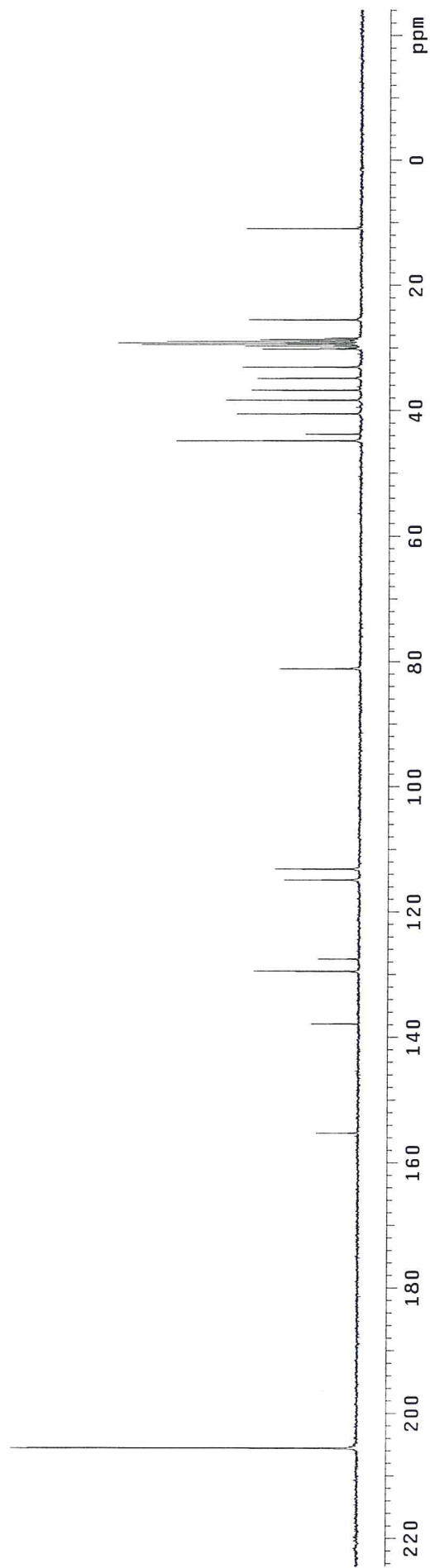
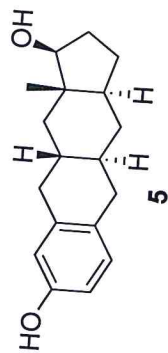
mq1261

Pulse Sequence: s2pu1

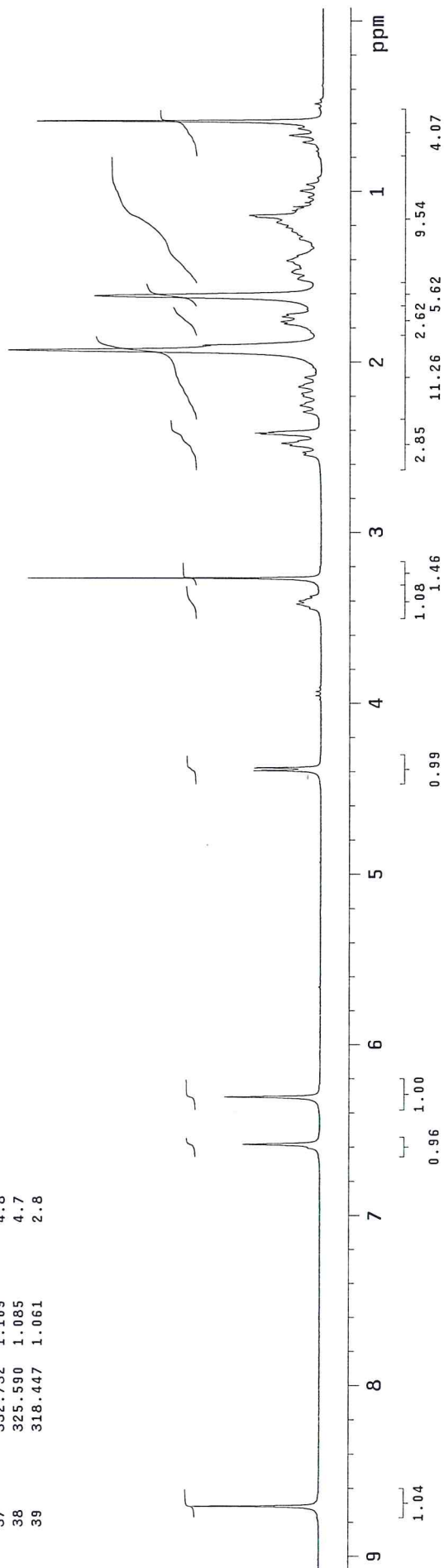
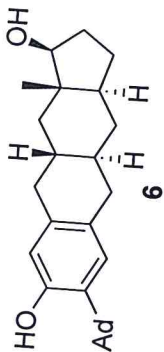


mq1261C

Pulse Sequence: s2pu1

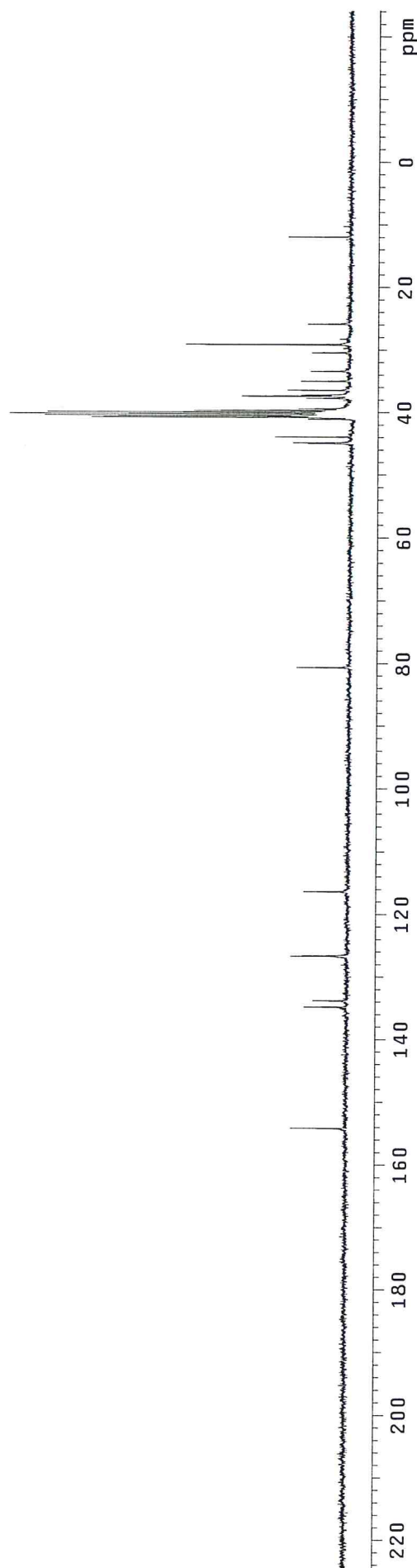
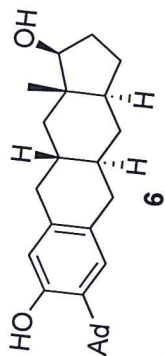


INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2611.938	8.705	20.3	40	309.107	1.030	2.2
2	1975.178	6.583	12.4	41	297.845	0.993	3.5
3	1891.943	6.305	15.3	42	286.307	0.954	2.5
4	1317.540	4.391	10.8	43	211.863	0.706	3.1
5	1312.870	4.376	10.7	44	200.050	0.667	5.3
6	1023.883	3.412	4.0	45	187.964	0.626	3.9
7	1019.213	3.397	3.6	46	174.778	0.582	45.4
8	1010.697	3.368	1.8				
9	979.107	3.263	46.8				
10	762.092	2.540	2.9				
11	757.696	2.525	3.0				
12	745.884	2.486	5.1				
13	741.764	2.472	6.4				
14	725.556	2.418	9.8				
15	723.908	2.413	10.7				
16	721.985	2.406	8.5				
17	686.549	2.288	2.9				
18	674.736	2.249	3.5				
19	653.584	2.178	3.2				
20	642.047	2.140	3.7				
21	625.839	2.086	2.7				
22	578.041	1.926	50.0				
23	569.251	1.897	19.0				
24	531.616	1.772	6.0				
25	527.771	1.759	6.6				
26	519.255	1.731	6.4				
27	515.409	1.718	5.7				
28	482.719	1.609	36.3				
29	452.777	1.509	3.9				
30	440.690	1.469	4.9				
31	420.637	1.402	5.7				
32	382.453	1.275	3.6				
33	361.576	1.205	5.8				
34	353.334	1.178	7.3				
35	343.445	1.145	10.6				
36	340.973	1.136	11.7				
37	332.732	1.109	4.8				
38	325.590	1.085	4.7				
39	318.447	1.061	2.8				



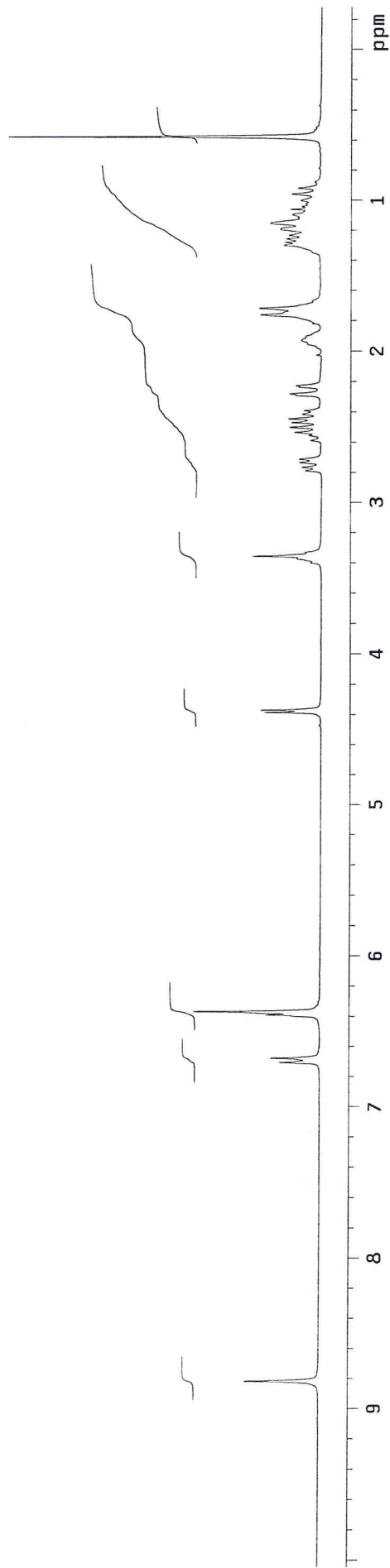
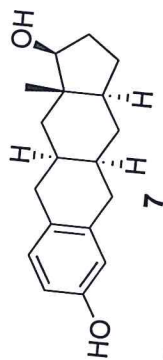
1262

INDEX	FREQUENCY	PPM	HEIGHT
1	11628.582	154.128	8.8
2	10168.459	134.776	6.8
3	10092.876	133.774	5.4
4	9553.489	126.625	9.0
5	9548.909	126.564	7.1
6	8775.902	116.318	6.9
7	6080.114	80.588	8.2
8	3386.616	44.887	6.7
9	3378.599	44.781	9.0
10	3307.597	43.840	11.9
11	3092.301	40.986	6.7
12	3071.687	40.713	41.2
13	3060.235	40.561	13.1
14	3051.073	40.440	48.7
15	3030.460	40.167	54.3
16	3008.701	39.878	48.3
17	2988.088	39.605	24.9
18	2967.474	39.332	8.2
19	2840.358	37.647	7.0
20	2815.163	37.313	17.2
21	2801.421	37.131	7.7
22	2743.016	36.357	9.9
23	2633.077	34.900	7.8
24	2512.832	33.306	6.3
25	2289.519	30.346	6.1
26	2192.177	29.056	26.2
27	1943.670	25.762	6.7
28	894.672	11.858	9.9



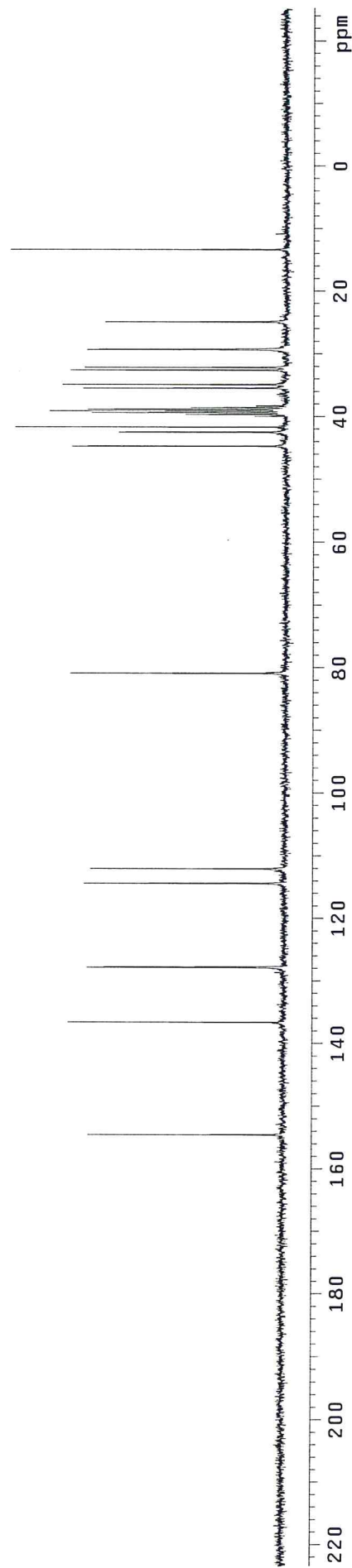
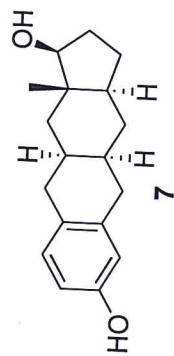
mq2072

Pu1se Sequence: s2pu1



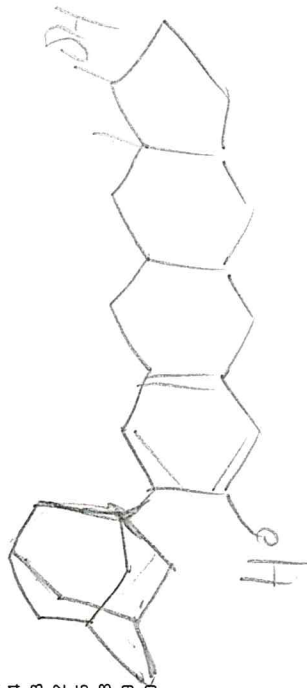
mq2072c

Pulse Sequence: s2pul

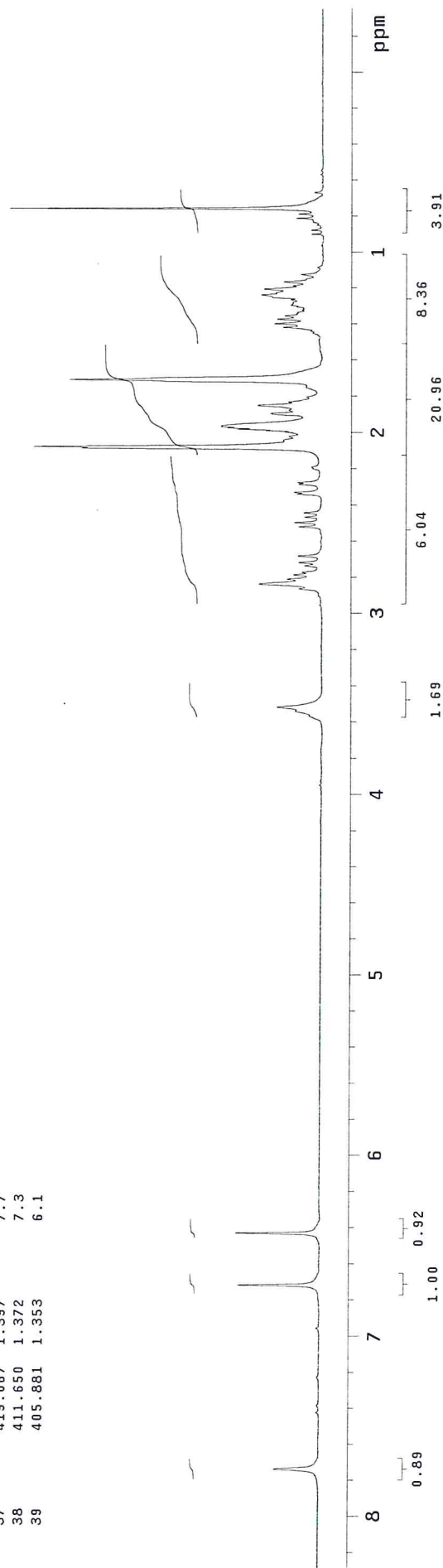
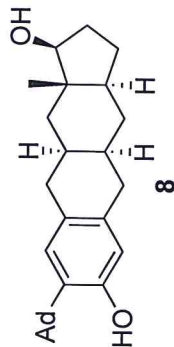


INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2322.206	7.739	7.2	40	400.113	1.333	4.1
2	2015.638	6.718	13.2	41	396.267	1.321	3.3
3	1929.381	6.430	13.6	42	390.773	1.302	4.2
4	1061.047	3.536	4.3	43	388.300	1.294	5.1
5	1055.003	3.516	7.2	44	378.961	1.263	5.2
6	858.316	2.861	3.7	45	370.719	1.236	9.8
7	850.899	2.836	10.1	46	367.972	1.226	7.5
8	842.384	2.807	5.6	47	361.105	1.203	9.4
9	835.516	2.785	4.5	48	355.886	1.186	4.8
10	830.846	2.769	3.2	49	349.018	1.163	6.2
11	820.133	2.733	2.8	50	336.656	1.122	3.5
12	814.639	2.715	3.8	51	242.708	0.809	4.3
13	803.925	2.679	3.9	52	235.566	0.785	3.9
14	755.303	2.517	3.8	53	226.501	0.755	50.0
15	748.435	2.494	4.5				
16	739.370	2.464	2.8				
17	732.228	2.440	2.9				
18	701.461	2.338	4.2				
19	698.439	2.328	4.5				
20	685.254	2.284	3.8				
21	682.232	2.274	4.0				
22	625.094	2.083	38.3				
23	622.622	2.075	46.1				
24	606.139	2.020	5.4				
25	598.722	1.995	6.1				
26	596.250	1.987	9.0				
27	594.053	1.980	13.7				
28	591.855	1.973	15.2				
29	589.383	1.964	16.2				
30	567.681	1.892	8.3				
31	562.462	1.875	5.4				
32	555.319	1.851	10.3				
33	549.276	1.831	5.5				
34	540.760	1.802	2.6				
35	512.191	1.707	40.3				
36	425.111	1.417	6.4				
37	419.067	1.397	7.7				
38	411.650	1.372	7.3				
39	405.881	1.353	6.1				

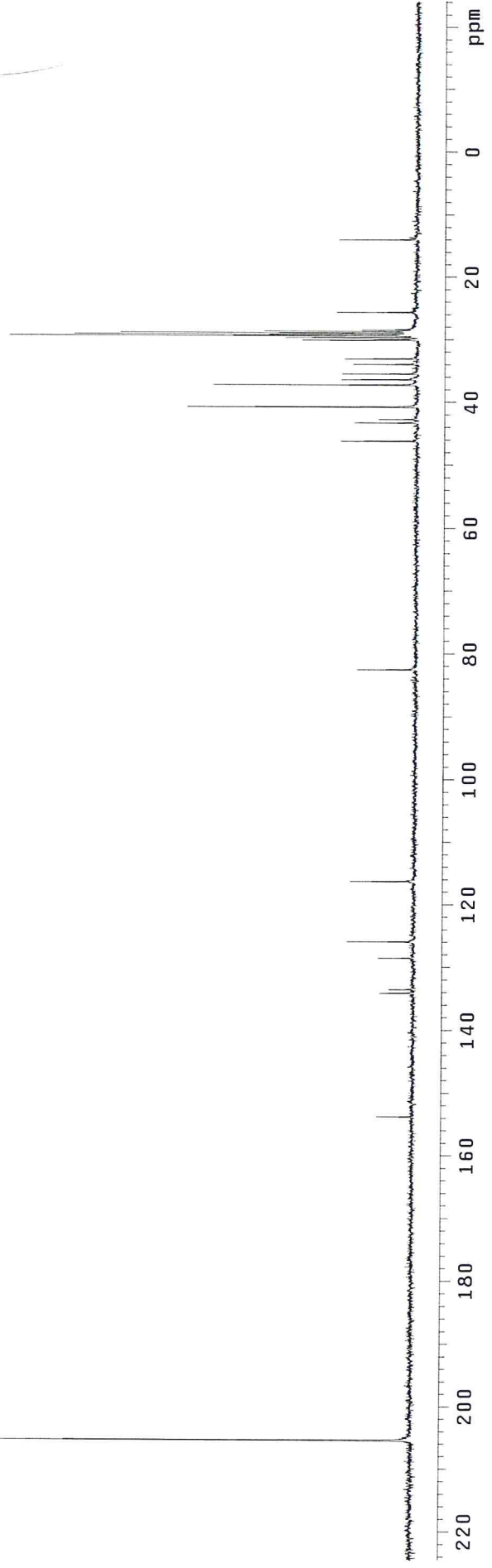
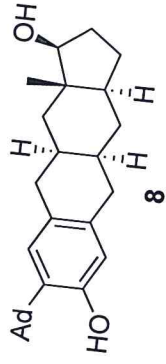
MQ 2075



acetone-d6

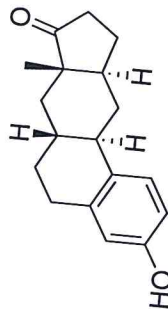


INDEX	FREQUENCY	PPM	HEIGHT
1	15499.344	205.433	82.8
2	11599.956	153.749	5.7
3	10115.783	134.077	5.3
4	10072.266	133.501	3.9
5	9694.352	128.492	5.6
6	9498.523	125.896	10.6
7	8770.179	116.242	10.2
8	6222.121	82.470	9.3
9	3481.670	46.147	12.0
10	3259.502	43.202	9.9
11	3218.275	42.656	6.0
12	3071.690	40.713	36.5
13	2806.005	37.192	32.5
14	2741.874	36.342	12.0
15	2672.017	35.416	11.9
16	2557.498	33.898	10.1
17	2489.931	33.002	11.5
18	2265.473	30.027	18.2
19	2254.021	29.875	6.8
20	2234.553	29.617	20.9
21	2213.939	29.344	65.0
22	2195.616	29.101	54.6
23	2176.148	28.843	47.3
24	2156.680	28.585	24.3
25	2137.211	28.327	8.8
26	1931.076	25.595	12.8
27	1050.421	13.923	12.4

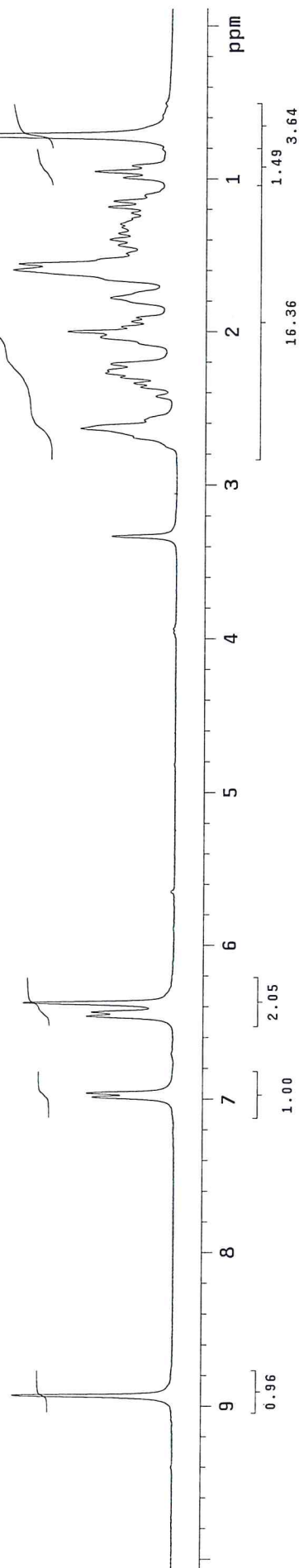


MQ1310

INDEX	FREQUENCY	PPM	HEIGHT
1	2680.614	8.934	25.7
2	2096.596	6.988	13.1
3	2088.904	6.962	14.0
4	1938.917	6.462	14.1
5	1930.676	6.435	13.3
6	1913.095	6.376	24.2
7	999.435	3.331	10.4
8	789.837	2.632	15.4
9	772.530	2.575	5.3
10	726.106	2.420	3.4
11	707.975	2.360	5.9
12	700.284	2.334	7.0
13	689.296	2.297	9.1
14	680.780	2.269	11.6
15	676.385	2.254	11.2
16	663.199	2.210	10.7
17	610.181	2.034	12.3
18	599.468	1.998	17.6
19	589.304	1.964	9.0
20	579.415	1.931	7.4
21	571.723	1.905	6.7
22	532.990	1.776	10.8
23	478.873	1.596	26.3
24	467.061	1.557	25.4
25	445.634	1.485	8.3
26	428.878	1.429	9.6
27	418.439	1.395	10.9
28	406.627	1.355	9.5
29	393.990	1.313	9.0
30	387.947	1.293	9.3
31	365.971	1.220	7.5
32	354.708	1.182	11.2
33	343.170	1.144	10.3
34	332.457	1.108	5.4
35	296.746	0.989	8.8
36	285.208	0.951	13.3
37	273.671	0.912	7.4
38	215.159	0.717	75.6



9



13C OBSERVE

Pulse Sequence: s2pul1

Solvent: DMSO

Ambient temperature

GEMINI-300BB "mbp-nmr"

Relax. delay 1.327 sec

Pulse 54.0 degrees

Acq. time 0.873 sec

Width 18761.7 Hz

320 repetitions

OBSERVE C13, 75.4473439 MHz

DECOUPLE H1, 300.0504026 MHz

Power 39 dB

continuously on

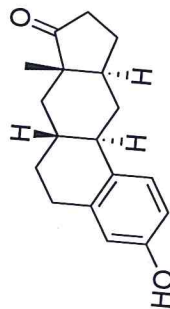
WALTZ-16 modulated

DATA PROCESSING

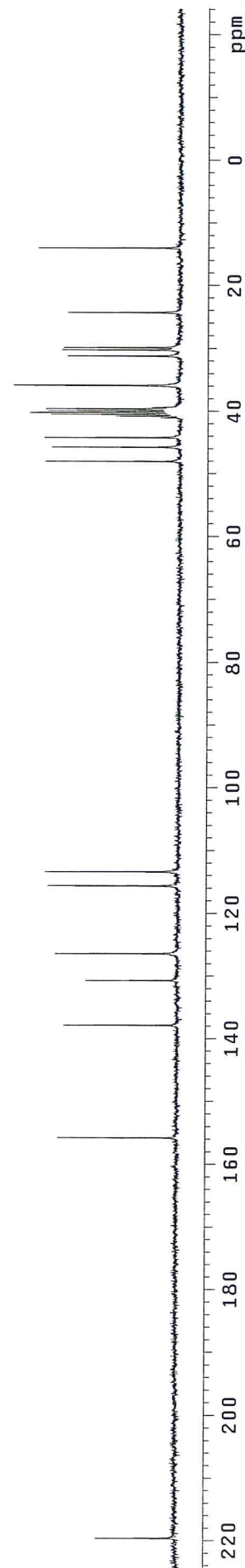
Line broadening 1.1 Hz

FT size 32768

Total time 0 min, 0 sec

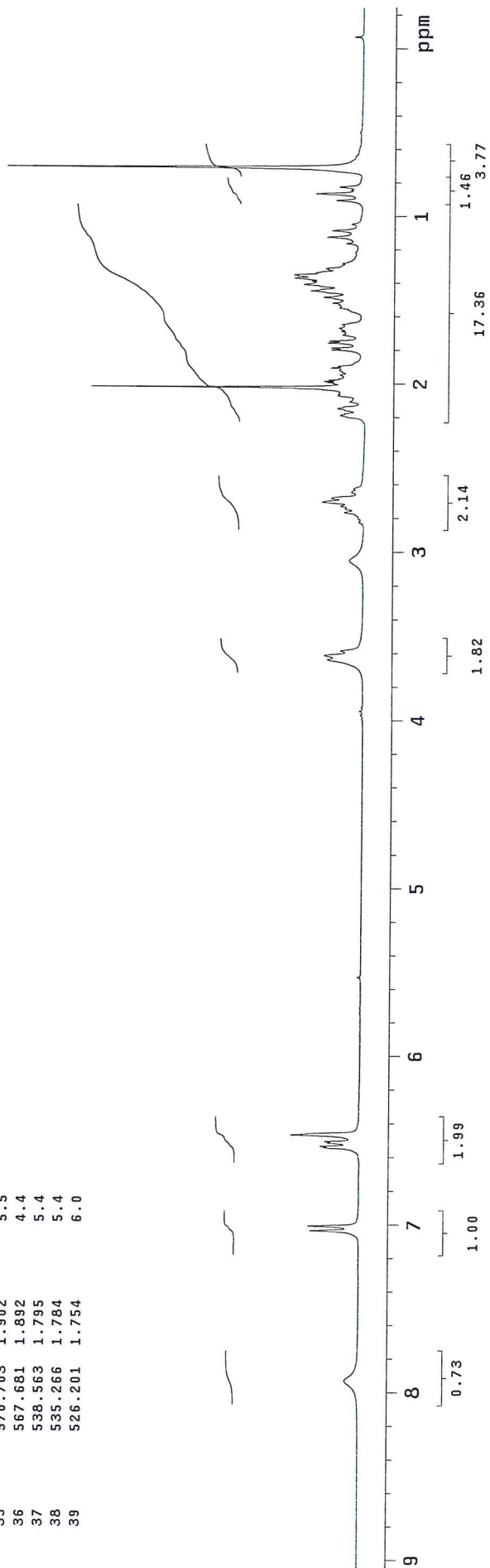
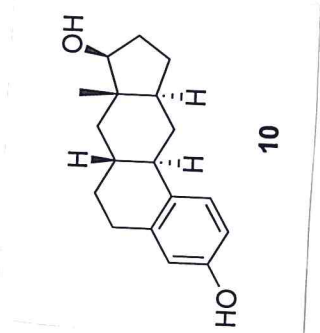


9



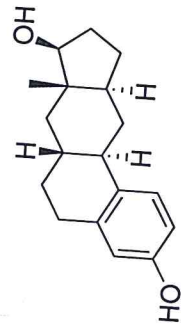
1311

mg	INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	40	522.905	1.743	5.8				
2	41	511.917	1.706	3.6				
3	42	509.719	1.699	3.3				
4	43	505.873	1.686	3.9				
5	44	502.027	1.673	3.9				
6	45	499.830	1.666	4.2				
7	46	495.709	1.652	3.4				
8	47	493.511	1.645	3.8				
9	48	463.844	1.546	4.2				
10	49	461.371	1.538	4.0				
11	50	458.624	1.528	4.3				
12	51	455.328	1.518	5.3				
13	52	444.889	1.483	6.7				
14	53	433.626	1.445	8.8				
15	54	422.089	1.407	9.9				
16	55	416.045	1.387	8.6				
17	56	410.551	1.368	11.3				
18	57	406.705	1.355	10.9				
19	58	405.057	1.350	11.4				
20	59	401.486	1.338	8.0				
21	60	395.717	1.319	6.0				
22	61	393.520	1.312	6.4				
23	62	384.729	1.282	3.7				
24	63	364.401	1.214	1.6				
25	64	348.469	1.161	3.2				
26	65	336.931	1.123	6.2				
27	66	325.394	1.084	5.4				
28	67	313.856	1.046	2.2				
29	68	271.002	0.903	4.8				
30	69	259.190	0.864	8.0				
31	70	252.872	0.843	2.5				
32	71	247.103	0.824	4.2				
33	72	211.941	0.706	57.3				
34	73	-21.556	-0.072	1.9				

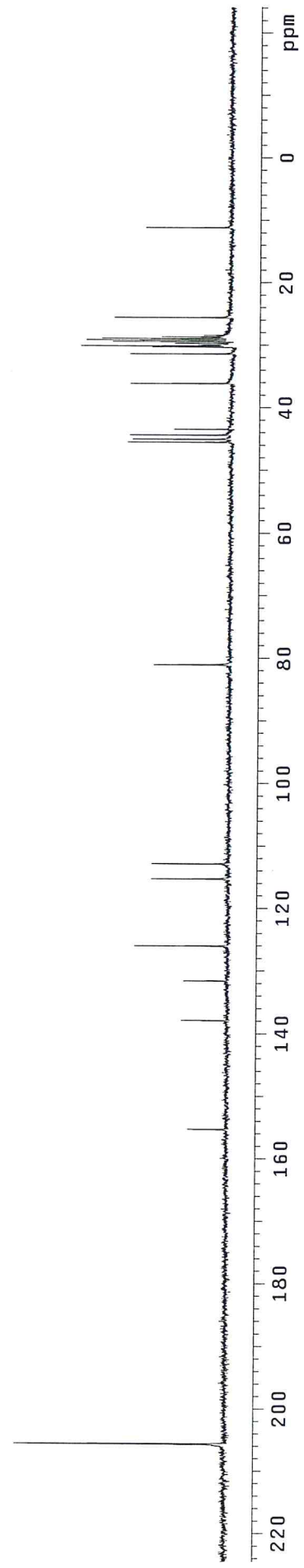


1311

INDEX	FREQUENCY	PPM	HEIGHT
1	15516.522	205.660	33.8
2	11714.475	155.267	6.2
3	10400.937	137.857	7.4
4	9925.681	131.558	7.1
5	9505.395	125.987	15.0
6	8694.597	115.241	12.4
7	8512.511	112.827	12.3
8	6113.328	81.028	12.2
9	3431.281	45.479	16.6
10	3396.926	45.024	15.8
11	3346.537	44.356	16.2
12	3275.535	43.415	9.1
13	2724.696	36.114	16.2
14	2366.250	31.363	16.3
15	2283.796	30.270	12.7
16	2271.199	30.103	24.1
17	2256.312	29.906	5.4
18	2237.988	29.663	9.2
19	2218.520	29.405	19.1
20	2199.052	29.147	23.2
21	2179.583	28.889	20.8
22	2160.115	28.631	11.2
23	2140.647	28.373	4.5
24	1927.641	25.549	18.8
25	840.851	11.145	13.8

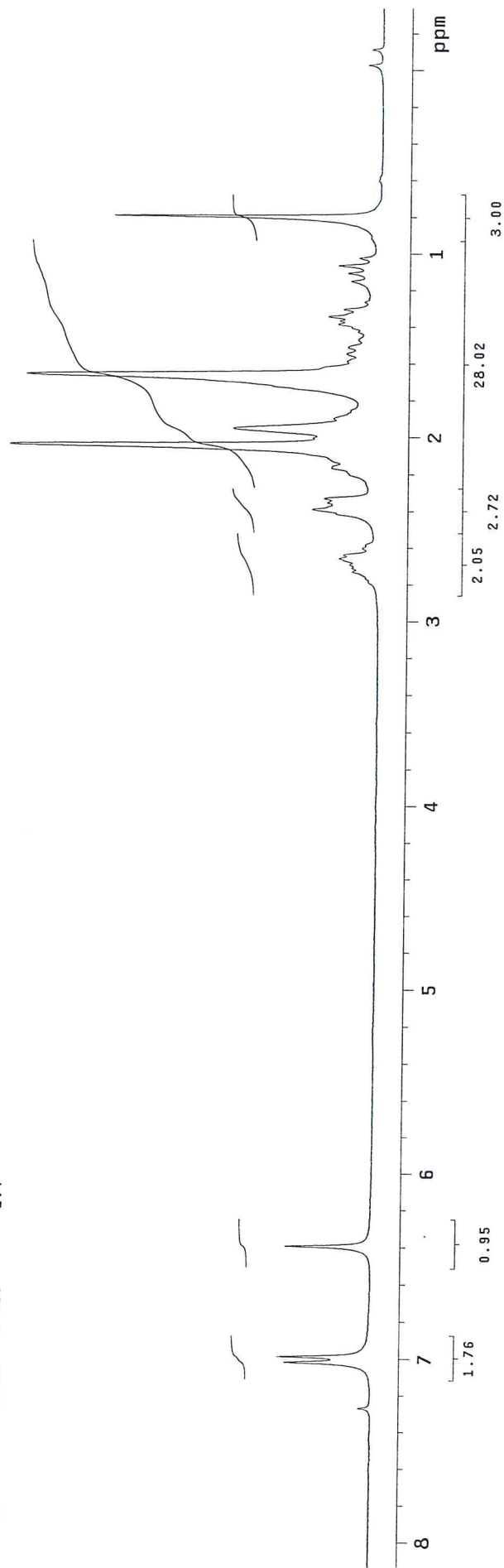
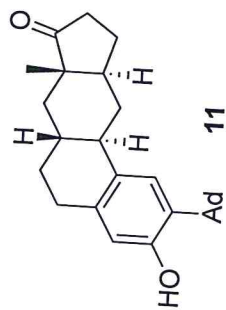
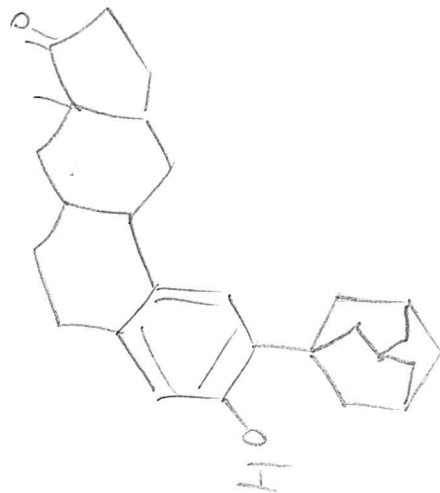


10



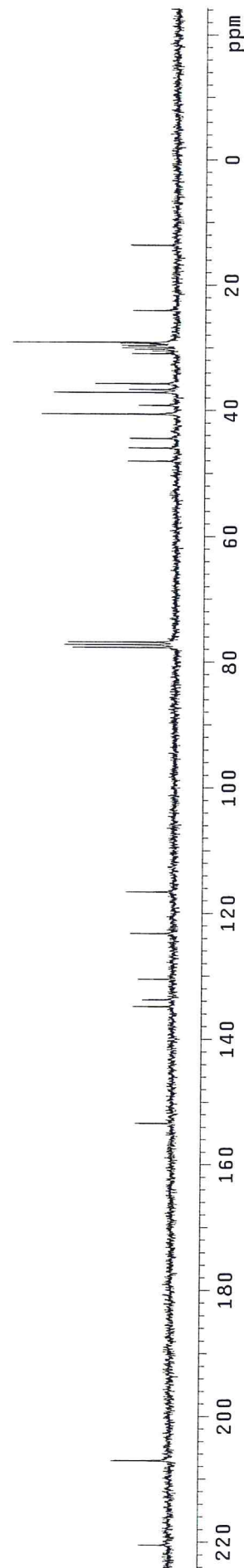
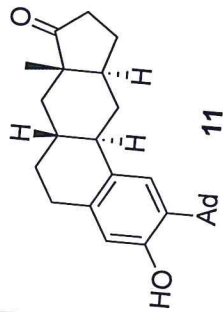
INDEX	FREQUENCY	PPM	HEIGHT
1	2106.363	7.020	13.8
2	2097.023	6.989	14.9
3	1918.741	6.395	13.8
4	818.283	2.727	4.2
5	811.965	2.706	4.3
6	806.471	2.688	4.6
7	795.208	2.650	6.0
8	796.856	2.656	6.3
9	791.088	2.637	5.7
10	780.374	2.601	2.6
11	716.643	2.388	10.7
12	705.655	2.352	8.3
13	698.513	2.328	8.8
14	649.341	2.164	7.7
15	613.355	2.044	59.2
16	600.993	2.003	10.8
17	585.885	1.953	23.4
18	568.579	1.895	7.4
19	498.804	1.662	56.6
20	476.279	1.587	5.4
21	463.368	1.544	5.4
22	453.204	1.510	5.2
23	441.117	1.470	3.6
24	415.020	1.383	6.8
25	409.251	1.364	6.5
26	402.658	1.342	8.4
27	390.846	1.303	6.0
28	378.210	1.260	2.6
29	344.971	1.150	4.8
30	331.510	1.105	5.3
31	318.874	1.063	6.9
32	306.787	1.022	3.5
33	238.661	0.795	42.7
34	-9.121	-0.030	2.4

CDCl₃-G2060



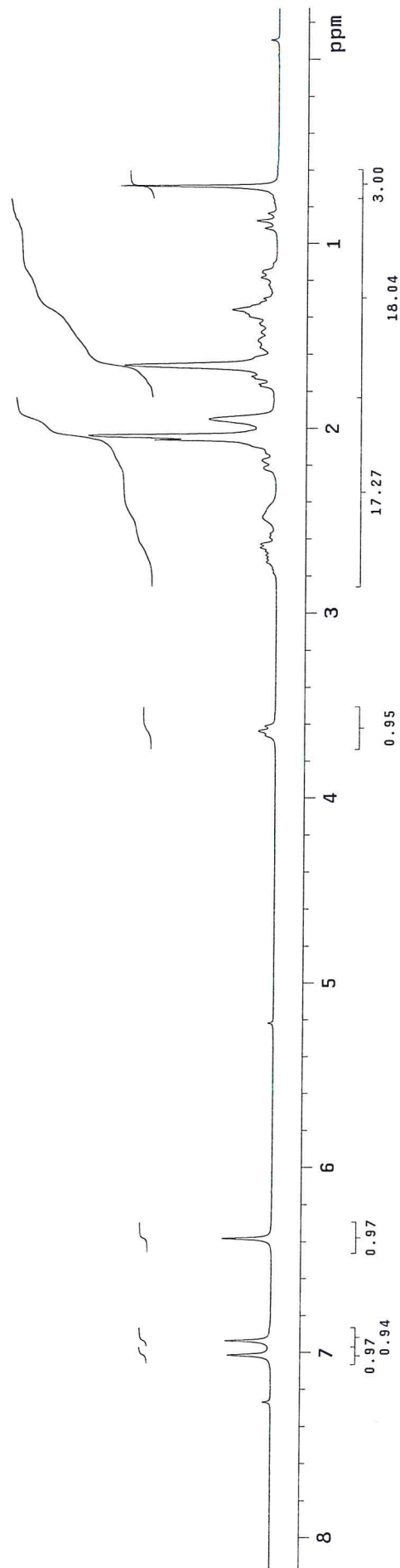
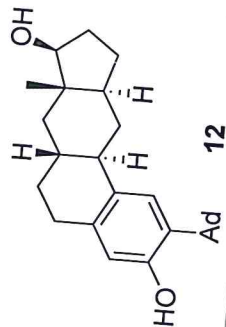
1313

INDEX	FREQUENCY	PPM	HEIGHT
1	16637.441	220.517	4.8
2	15625.088	207.099	9.3
3	11571.099	153.366	5.8
4	10171.871	134.818	6.4
5	10090.362	133.740	4.8
6	9844.145	130.477	5.6
7	9294.452	123.191	6.8
8	8794.002	116.558	7.6
9	5857.722	77.640	16.3
10	5825.657	77.215	17.7
11	5793.591	76.790	17.1
12	3621.157	47.996	7.6
13	3464.265	45.916	7.6
14	3349.746	44.398	7.4
15	3057.721	40.528	21.4
16	2951.218	39.116	6.0
17	2796.617	37.067	19.5
18	2761.115	36.597	7.5
19	2690.113	35.655	12.9
20	2329.377	30.874	7.1
21	2296.166	30.434	3.9
22	2276.698	30.176	6.7
23	2257.230	29.918	8.7
24	2237.761	29.660	7.8
25	2230.890	29.569	8.8
26	2206.841	29.250	9.0
27	2193.099	29.068	26.1
28	1809.459	23.983	7.0
29	1022.710	13.555	7.4



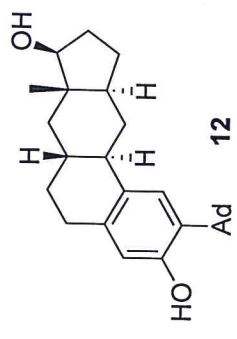
1312

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2181.345	7.270	1.3	40	231.782	0.772	0.8
2	2104.978	7.015	7.0	41	205.685	0.686	25.3
3	2081.353	6.937	7.4	42	-32.207	-0.107	1.4
4	1915.158	6.383	8.0				
5	1565.462	5.217	0.9				
6	1097.919	3.659	1.7				
7	1090.227	3.634	2.8				
8	1082.535	3.608	1.8				
9	817.448	2.724	1.7				
10	811.129	2.703	1.6				
11	805.910	2.686	1.8				
12	799.867	2.666	1.9				
13	793.823	2.646	2.7				
14	787.780	2.626	2.6				
15	776.517	2.588	1.2				
16	771.572	2.572	1.1				
17	744.377	2.481	2.3				
18	664.164	2.214	2.2				
19	651.527	2.171	2.5				
20	618.838	2.062	19.7				
21	612.245	2.040	30.3				
22	584.775	1.949	11.0				
23	530.933	1.769	2.9				
24	527.636	1.759	3.1				
25	518.846	1.729	3.8				
26	515.550	1.718	4.3				
27	498.243	1.661	24.6				
28	468.026	1.560	3.0				
29	457.587	1.525	3.2				
30	443.852	1.479	2.7				
31	429.018	1.430	3.1				
32	407.591	1.358	7.4				
33	388.637	1.295	2.4				
34	366.111	1.220	1.6				
35	354.849	1.183	2.8				
36	346.333	1.154	2.7				
37	274.361	0.914	2.2				
38	262.274	0.874	3.6				
39	250.187	0.834	1.8				

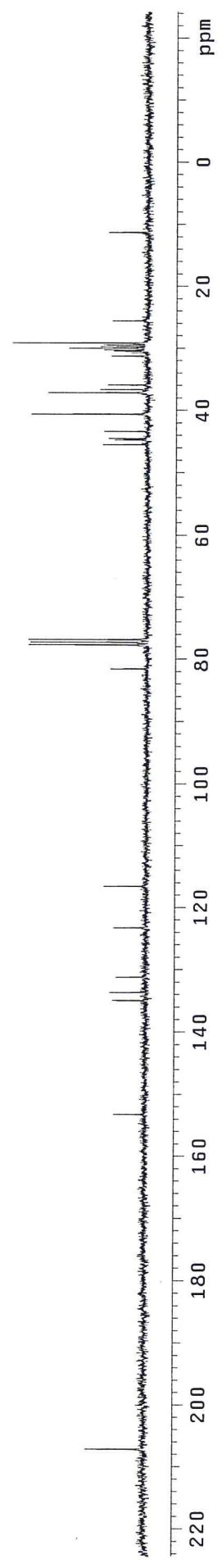


1312

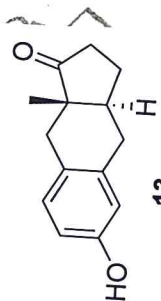
INDEX	FREQUENCY	PPM	HEIGHT
1	15630.784	207.176	9.4
2	11557.326	153.185	5.1
3	10178.512	134.909	5.4
4	10081.170	133.619	5.8
5	9896.794	131.175	4.8
6	9295.566	123.207	5.3
7	8790.536	116.513	6.9
8	6148.571	81.495	5.9
9	5857.692	77.640	19.1
10	5825.626	77.215	18.8
11	5793.561	76.790	19.1
12	3427.588	45.430	7.2
13	3370.329	44.671	5.3
14	3353.151	44.444	6.3
15	3266.116	43.290	7.0
16	3058.836	40.543	18.8
17	2798.876	37.097	16.1
18	2759.940	36.581	7.7
19	2704.970	35.853	6.4
20	2353.396	31.193	5.8
21	2297.281	30.449	3.7
22	2289.265	30.343	5.5
23	2277.813	30.191	7.1
24	2258.344	29.933	12.7
25	2238.876	29.675	7.6
26	2218.263	29.402	7.2
27	2194.214	29.083	21.8
28	1925.093	25.516	5.7
29	846.319	11.217	6.4



12

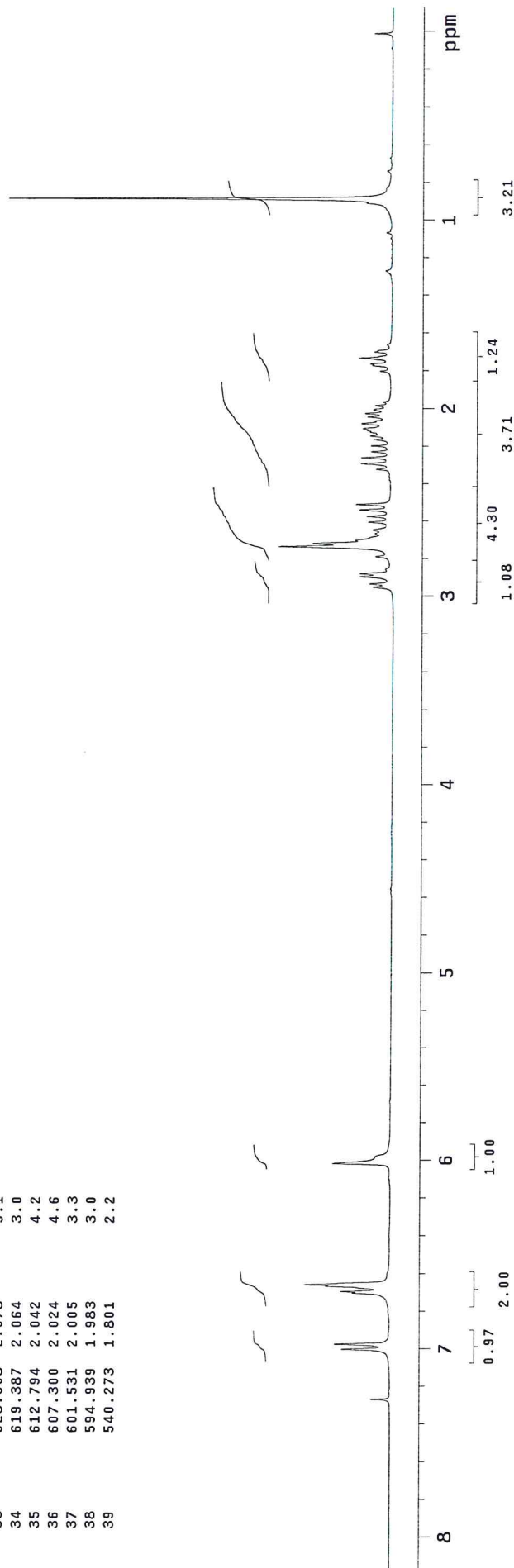


MQ 1042

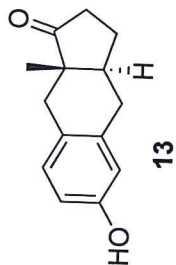


13

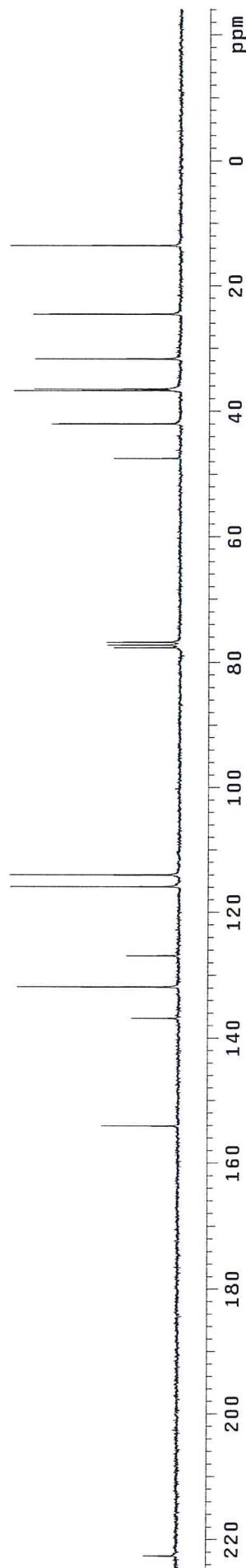
INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2181.345	7.270	3.2	40	531.208	1.770	3.5
2	2101.407	7.004	7.9	41	528.735	1.762	3.8
3	2093.440	6.977	9.0	42	519.670	1.732	5.6
4	2011.304	6.703	6.3	43	509.781	1.699	3.1
5	2009.107	6.696	8.1	44	508.133	1.694	2.6
6	2000.591	6.668	10.5	45	272.163	0.907	4.5
7	1998.119	6.659	13.9	46	265.021	0.883	61.8
8	1805.277	6.017	9.4	47	2.955	0.010	3.2
9	885.299	2.951	3.2				
10	879.805	2.932	3.7				
11	868.542	2.895	5.4				
12	863.598	2.878	5.4				
13	836.402	2.788	2.8				
14	820.469	2.734	18.4				
15	815.799	2.719	12.9				
16	810.305	2.701	6.1				
17	799.592	2.665	2.9				
18	793.823	2.646	3.3				
19	781.187	2.604	4.0				
20	772.122	2.573	4.3				
21	761.683	2.539	5.5				
22	752.892	2.509	6.1				
23	696.304	2.321	2.8				
24	687.513	2.291	5.2				
25	677.899	2.259	5.2				
26	668.284	2.227	3.6				
27	658.944	2.196	3.6				
28	649.055	2.163	3.2				
29	643.011	2.143	3.8				
30	636.968	2.123	3.8				
31	634.221	2.114	4.3				
32	631.199	2.104	4.9				
33	623.508	2.078	5.1				
34	619.387	2.064	3.0				
35	612.794	2.042	4.2				
36	607.300	2.024	4.6				
37	601.531	2.005	3.3				
38	594.939	1.983	3.0				
39	540.273	1.801	2.2				



1042

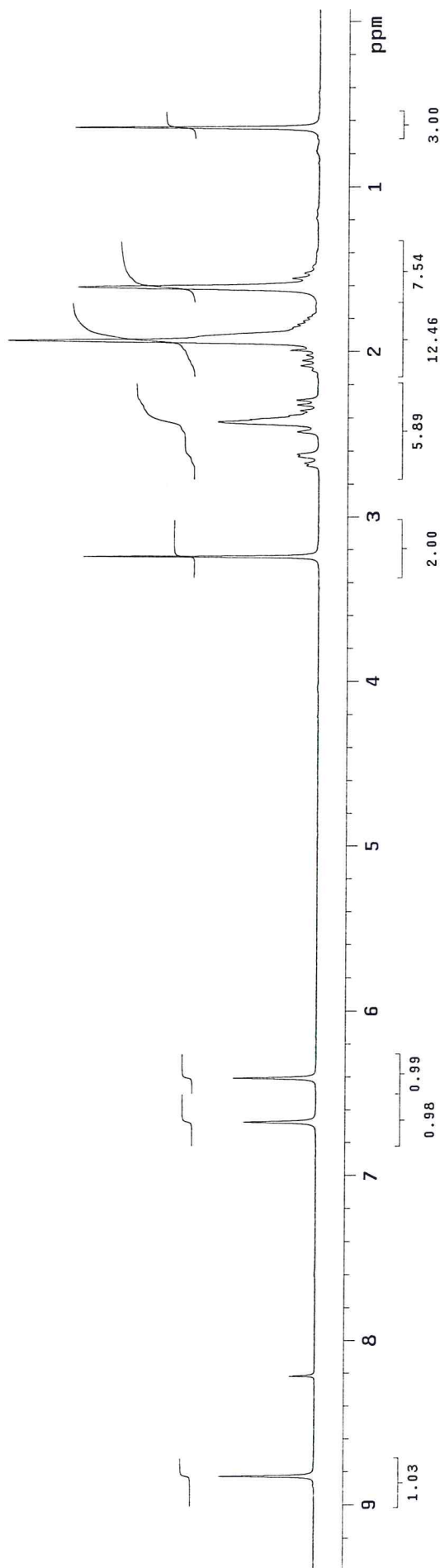
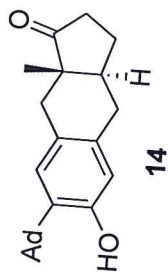
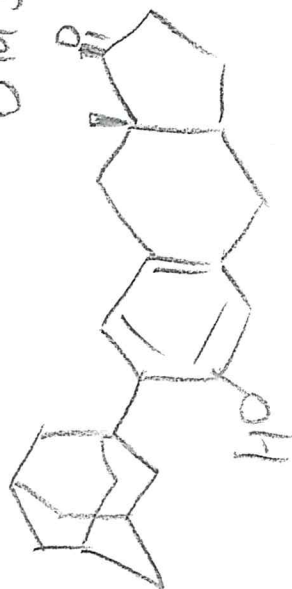


INDEX	FREQUENCY	PPM	HEIGHT
1	16796.592	222.628	5.4
2	11621.456	154.035	12.4
3	10320.515	136.792	7.6
4	9942.601	131.783	26.0
5	9569.267	126.834	8.5
6	8740.146	115.845	27.2
7	8598.142	113.963	27.3
8	5856.546	77.625	10.6
9	5824.480	77.200	11.7
10	5792.415	76.775	11.8
11	3576.463	47.404	10.7
12	3163.048	41.924	20.8
13	2765.665	36.657	26.8
14	2746.197	36.399	23.6
15	2385.460	31.618	23.4
16	1847.219	24.484	23.7
17	1016.953	13.479	27.4



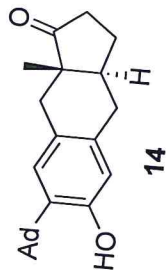
INDEX	FREQUENCY	PPM	HEIGHT
1	2649.297	8.830	15.5
2	2466.071	8.219	4.1
3	2002.648	6.674	11.7
4	1922.435	6.407	13.4
5	973.063	3.243	37.7
6	805.495	2.685	2.0
7	801.099	2.670	2.4
8	789.013	2.630	3.4
9	785.441	2.618	3.5
10	744.511	2.481	3.5
11	726.930	2.423	16.2
12	723.084	2.410	11.2
13	706.602	2.355	3.0
14	696.163	2.320	3.5
15	687.647	2.292	3.6
16	625.015	2.083	3.1
17	615.675	2.052	2.7
18	606.061	2.020	2.1
19	597.545	1.991	4.7
20	580.513	1.935	50.0
21	549.747	1.832	3.6
22	544.253	1.814	2.6
23	537.934	1.793	2.0
24	483.269	1.611	38.8
25	466.512	1.555	4.3
26	456.348	1.521	2.4
27	192.908	0.643	39.3

1044 DMSO

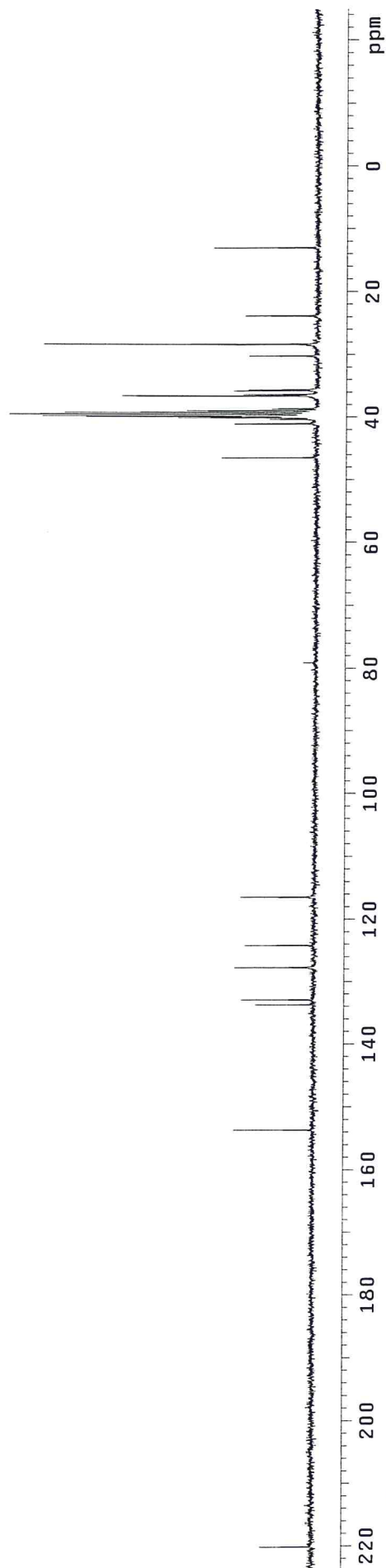


1044

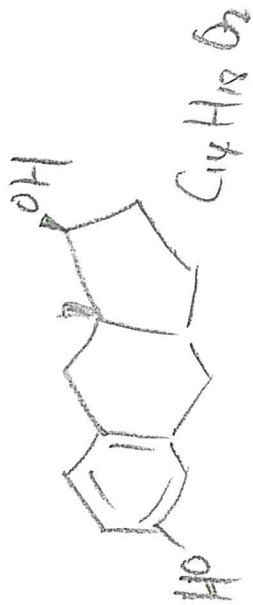
INDEX	FREQUENCY	PPM	HEIGHT
1	16613.325	220.197	8.2
2	11595.082	153.684	13.0
3	10090.296	133.739	9.3
4	10030.746	132.950	11.8
5	9639.089	127.759	13.0
6	9371.113	124.207	11.2
7	8788.209	116.481	12.0
8	3506.571	46.477	15.4
9	3097.736	41.058	13.3
10	3043.912	40.345	7.4
11	3022.154	40.056	22.4
12	3010.702	39.905	37.2
13	3001.540	39.783	44.3
14	2980.927	39.510	49.5
15	2959.168	39.222	40.7
16	2938.554	38.948	21.0
17	2917.941	38.675	7.1
18	2761.049	36.596	31.4
19	2743.871	36.368	11.9
20	2698.063	35.761	13.5
21	2686.612	35.609	11.0
22	2281.213	30.236	10.9
23	2139.208	28.354	44.0
24	1800.231	23.861	11.6
25	983.707	13.038	16.8



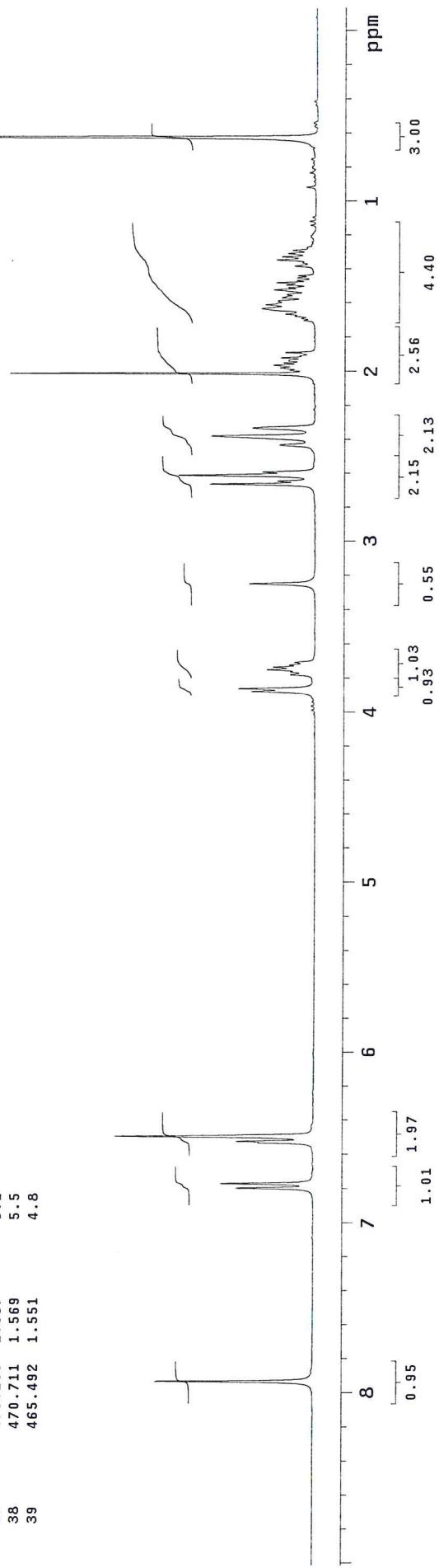
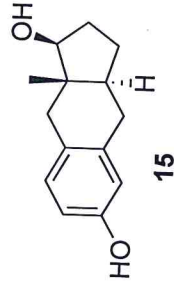
14



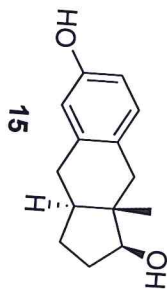
INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2380.992	7.935	25.5	40	456.976	1.523	6.8
2	2039.811	6.798	12.6	41	452.855	1.509	4.6
3	2031.845	6.772	15.0	42	447.911	1.493	4.9
4	1960.422	6.534	9.0	43	444.065	1.480	6.5
5	1957.950	6.525	12.5	44	440.219	1.467	3.2
6	1949.434	6.497	32.1	45	435.275	1.451	3.1
7	1163.511	3.878	10.3	46	431.703	1.439	3.0
8	1158.566	3.861	12.4	47	414.672	1.382	3.5
9	1133.568	3.778	4.1	48	403.958	1.346	6.4
10	1128.623	3.761	4.1	49	398.464	1.328	5.6
11	1125.052	3.750	7.8	50	392.146	1.307	4.6
12	1120.382	3.734	6.8	51	386.927	1.290	3.8
13	1116.262	3.720	4.3	52	186.944	0.623	100.0
14	1111.867	3.706	3.4				
15	974.515	3.248	10.7				
16	798.981	2.663	17.1				
17	793.487	2.645	6.2				
18	783.323	2.611	22.1				
19	777.279	2.591	8.6				
20	729.481	2.431	5.9				
21	713.823	2.379	16.9				
22	699.538	2.331	10.3				
23	603.942	2.013	49.2				
24	597.624	1.992	4.3				
25	593.228	1.977	5.8				
26	588.833	1.962	6.9				
27	584.987	1.950	5.3				
28	580.043	1.933	4.5				
29	575.647	1.919	5.7				
30	572.626	1.908	2.7				
31	566.857	1.889	5.0				
32	507.247	1.691	2.4				
33	503.126	1.677	3.5				
34	499.555	1.665	5.0				
35	490.215	1.634	8.8				
36	483.347	1.611	8.2				
37	476.205	1.587	6.2				
38	470.711	1.569	5.5				
39	465.492	1.551	4.8				



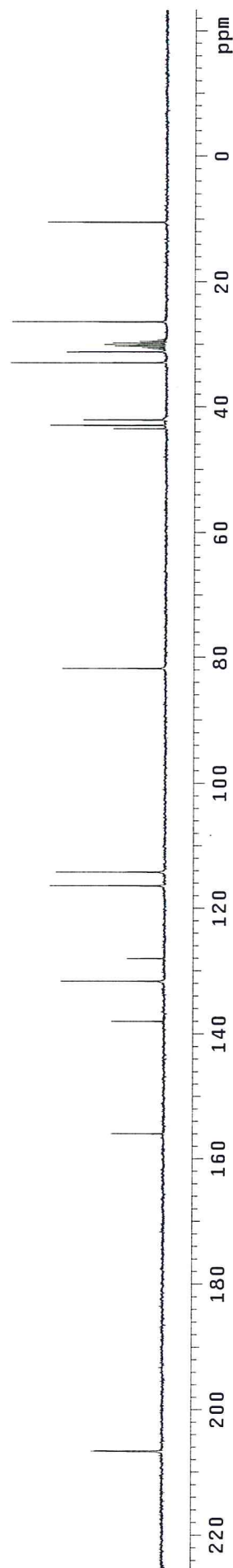
in acetone-d₆



1047

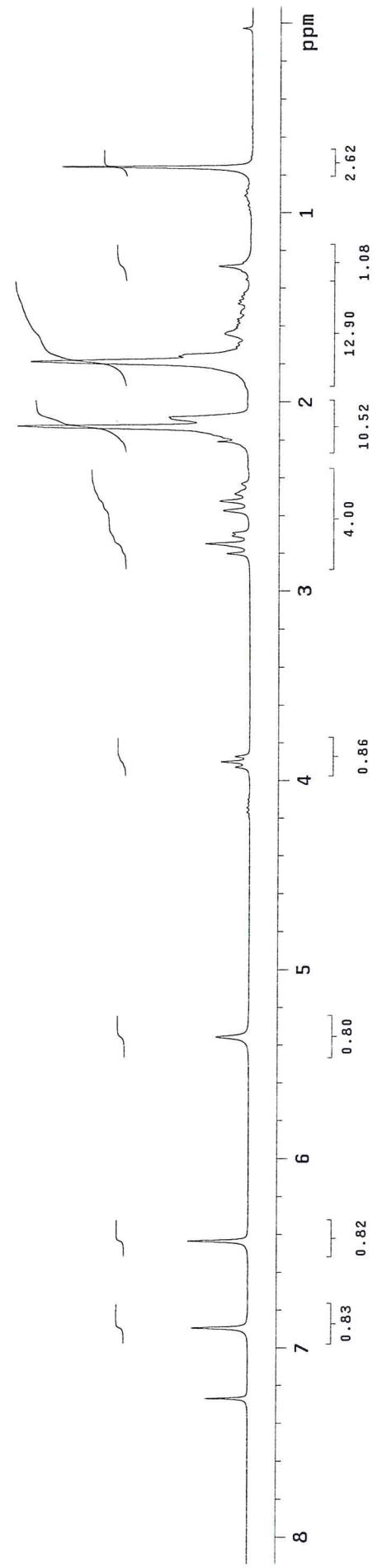
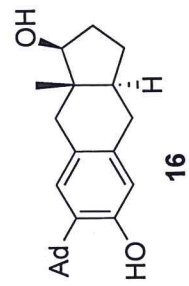
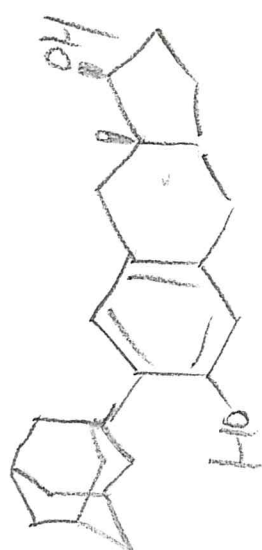


INDEX	FREQUENCY	PPM	HEIGHT
1	15592.307	206.665	11.5
2	11765.066	155.937	8.5
3	10410.300	137.981	8.5
4	9929.318	131.606	16.7
5	9656.762	127.993	6.1
6	8779.543	116.367	18.5
7	8613.490	114.166	17.5
8	6166.208	81.729	16.6
9	3276.882	43.433	8.5
10	3236.800	42.901	18.6
11	3171.524	42.036	13.3
12	2480.972	32.883	25.0
13	2350.419	31.153	16.1
14	2298.886	30.470	4.0
15	2279.417	30.212	8.3
16	2259.949	29.954	10.0
17	2240.481	29.696	8.7
18	2221.012	29.438	4.3
19	1987.393	26.341	24.8
20	786.083	10.419	19.1

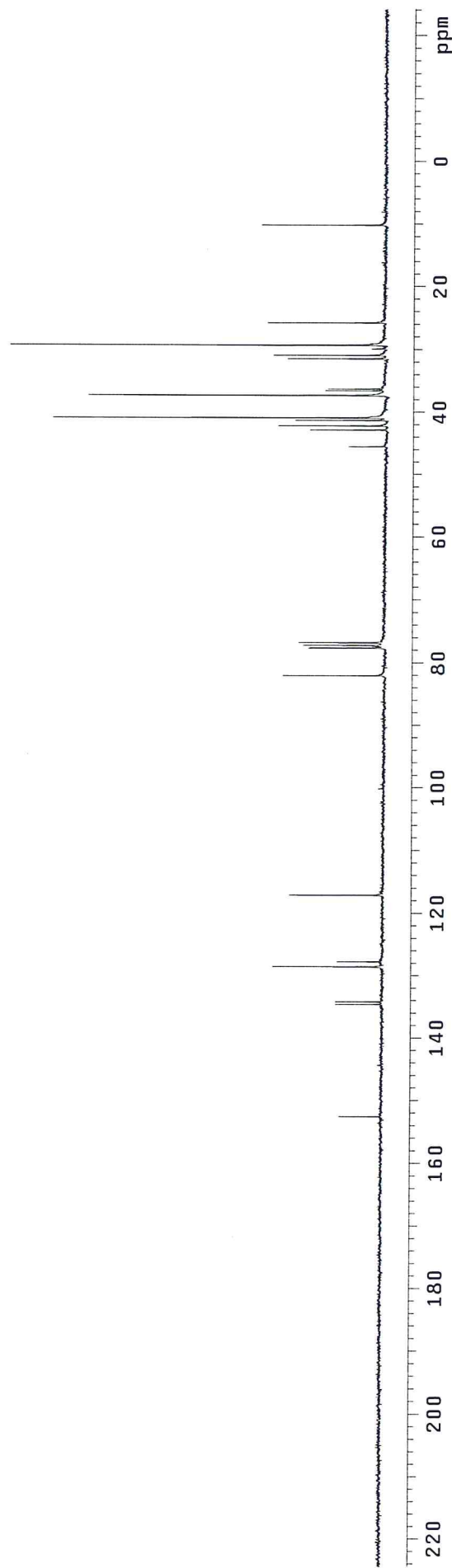
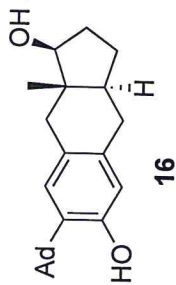


MO-1045

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2181.345	7.270	6.8	21	513.077	1.710	2.4
2	2068.717	6.895	9.1	22	507.308	1.691	2.2
3	1930.542	6.434	9.7	23	492.200	1.640	4.2
4	1607.217	5.357	5.2	24	481.212	1.604	2.4
5	1178.407	3.927	2.4	25	477.366	1.591	2.3
6	1170.165	3.900	4.6	26	472.696	1.575	2.2
7	1161.375	3.871	2.4	27	468.575	1.562	2.3
8	839.973	2.799	3.8	28	459.236	1.531	1.8
9	824.590	2.748	7.2	29	443.852	1.479	2.2
10	811.953	2.706	3.0	30	438.908	1.463	2.0
11	807.284	2.691	2.9	31	432.589	1.442	1.6
12	771.572	2.572	4.4	32	427.095	1.423	1.2
13	756.464	2.521	5.0	33	405.394	1.351	0.9
14	745.201	2.484	2.5	34	384.516	1.282	5.2
15	728.719	2.429	1.5	35	378.473	1.261	1.4
16	661.966	2.206	5.4	36	272.163	0.907	1.1
17	638.067	2.127	37.5	37	264.197	0.881	0.9
18	623.508	2.078	13.2	38	226.837	0.756	30.4
19	536.702	1.789	35.4	39	7.350	0.024	1.5
20	527.911	1.759	11.7				

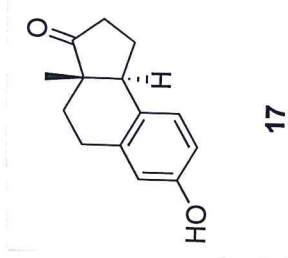


INDEX	FREQUENCY	PPM	HEIGHT
1	11509.454	152.550	6.8
2	10154.689	134.594	7.5
3	10123.769	134.184	7.5
4	9698.901	128.553	17.6
5	9638.206	127.748	7.3
6	8833.134	117.077	15.0
7	6187.734	82.014	16.3
8	5855.628	77.612	12.1
9	5823.562	77.187	12.9
10	5791.497	76.762	13.7
11	3430.105	45.464	5.8
12	3229.696	42.807	12.0
13	3180.453	42.155	17.1
14	3112.886	41.259	14.4
15	3084.256	40.880	53.3
16	2812.845	37.282	47.6
17	2754.440	36.508	9.6
18	2733.827	36.235	9.2
19	2369.655	31.408	15.7
20	2328.428	30.862	17.9
21	2208.182	29.268	60.2
22	1940.207	25.716	18.9
23	764.092	10.128	19.9

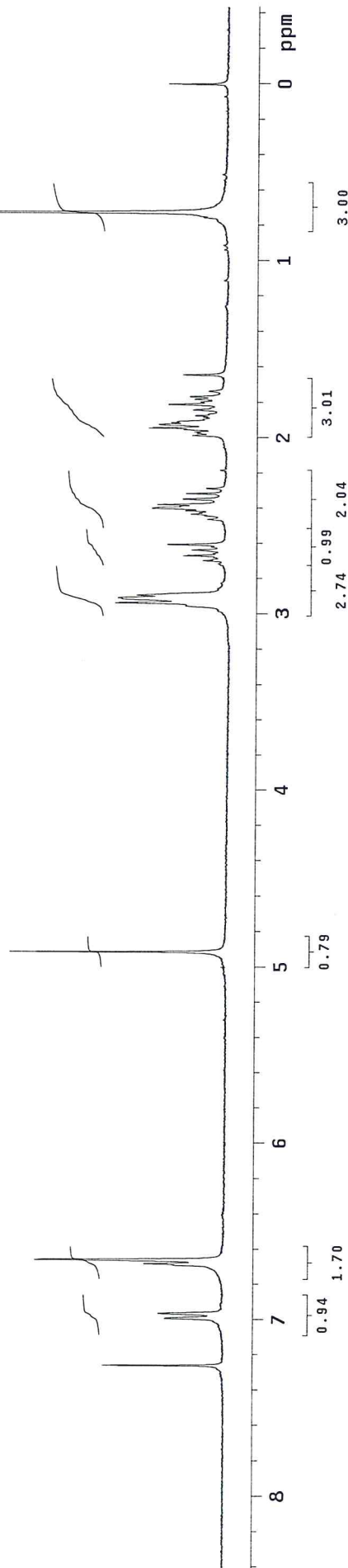


MQ1022

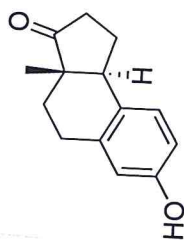
INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2179.489	7.264	18.0	40	-0.000	-0.000	9.8
2	2178.940	7.262	19.5				
3	2099.001	6.996	9.5				
4	2090.211	6.966	10.5				
5	2005.603	6.684	12.9				
6	1999.010	6.662	30.4				
7	1474.328	4.914	34.7				
8	881.245	2.937	18.0				
9	872.730	2.909	17.6				
10	868.609	2.895	14.6				
11	809.273	2.697	4.0				
12	800.758	2.669	7.3				
13	791.143	2.637	5.8				
14	781.803	2.606	9.7				
15	738.950	2.463	3.4				
16	729.884	2.433	6.0				
17	724.116	2.413	6.9				
18	720.270	2.401	12.2				
19	713.677	2.379	11.4				
20	704.337	2.347	7.3				
21	694.722	2.315	6.8				
22	686.207	2.287	3.5				
23	595.830	1.986	5.8				
24	592.533	1.975	5.1				
25	589.786	1.966	5.5				
26	583.193	1.944	12.8				
27	577.150	1.924	11.2				
28	574.403	1.914	9.2				
29	564.788	1.882	4.0				
30	562.041	1.873	5.4				
31	552.427	1.841	5.7				
32	543.361	1.811	9.7				
33	538.966	1.796	4.5				
34	534.296	1.781	5.5				
35	529.901	1.766	6.2				
36	520.836	1.736	3.2				
37	493.091	1.643	7.3				
38	218.114	0.727	100.0				
39	0.824	0.003	7.6				



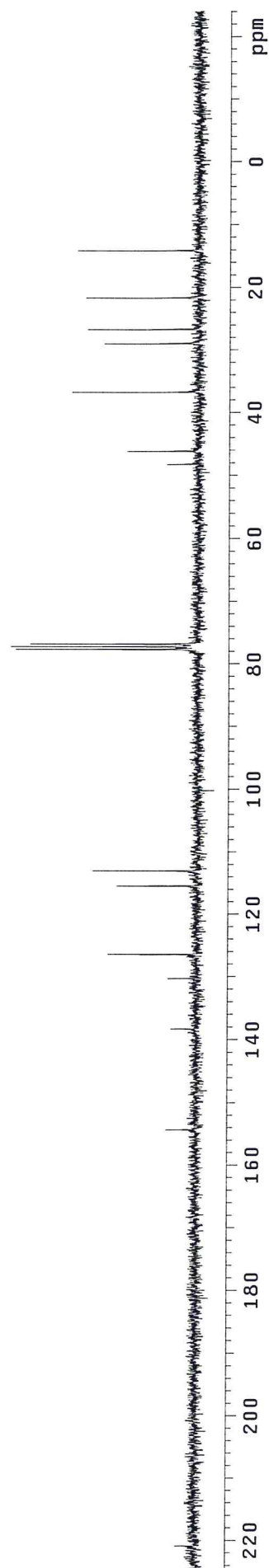
17



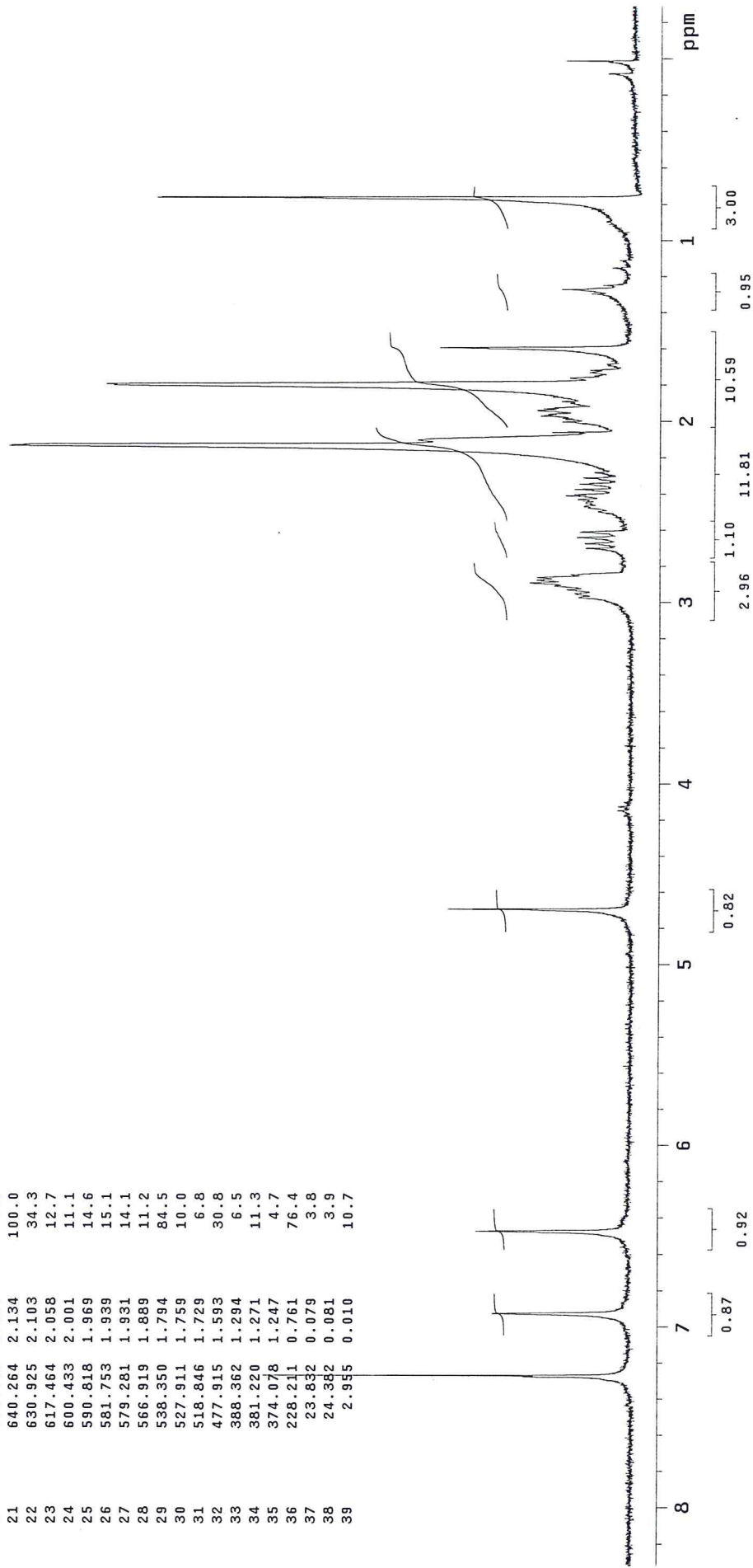
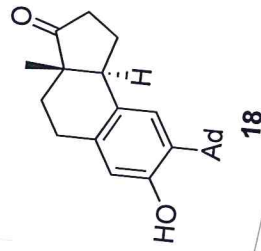
INDEX	FREQUENCY	PPM	HEIGHT
1	16659.168	220.806	3.1
2	11640.924	154.293	5.0
3	10433.889	138.294	4.2
4	9828.081	130.255	4.8
5	9537.201	126.409	14.6
6	8709.226	115.435	13.3
7	8524.849	112.991	17.1
8	7560.595	100.211	-2.7
9	5857.691	77.640	29.6
10	5825.625	77.215	30.4
11	5793.560	76.790	27.3
12	3638.303	48.223	5.3
13	3481.411	46.144	11.8
14	2771.391	36.733	20.7
15	2185.051	28.961	15.5
16	2013.272	26.685	18.2
17	1633.067	21.645	18.5
18	1063.905	14.101	19.9



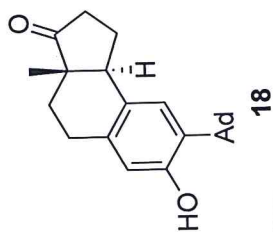
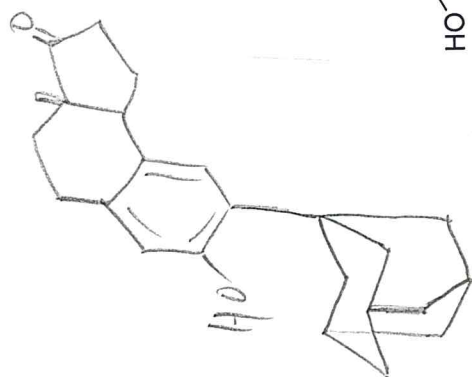
17



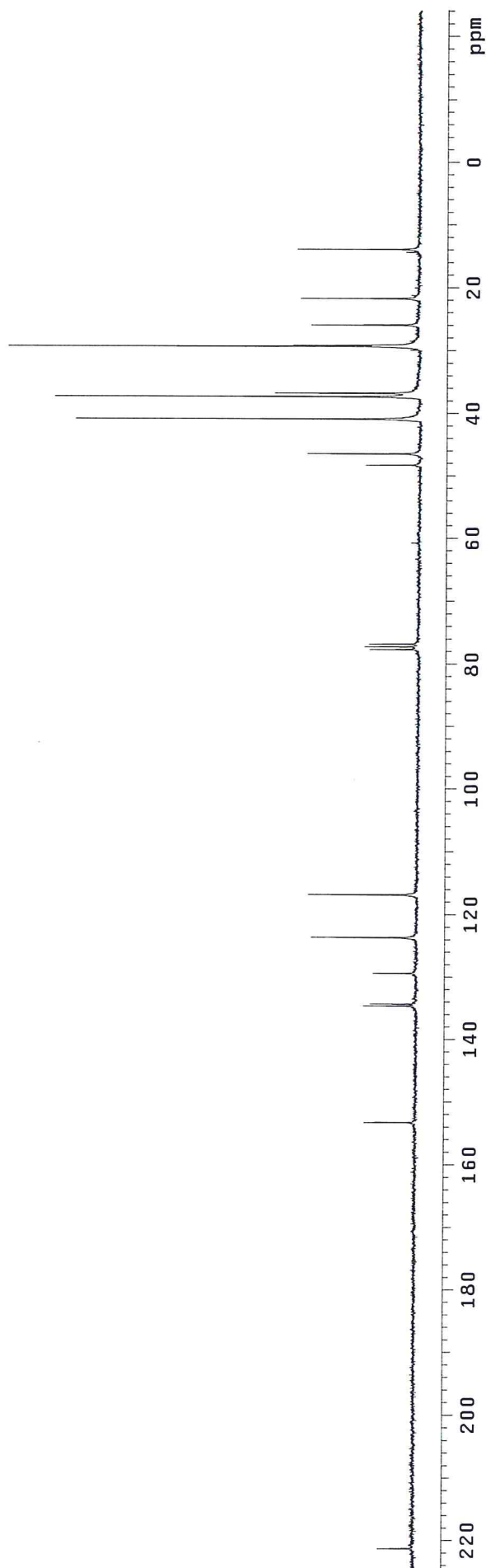
INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2181.345	7.270	58.8	20	683.942	2.279	5.9
2	2078.332	6.927	21.9	21	640.264	2.134	100.0
3	1942.354	6.473	24.6	22	630.925	2.103	34.3
4	1408.607	4.695	29.3	23	617.464	2.058	12.7
5	884.475	2.948	9.1	24	600.433	2.001	11.1
6	878.431	2.928	10.4	25	590.818	1.969	14.6
7	867.443	2.891	16.3	26	581.753	1.939	15.1
8	862.499	2.875	15.2	27	579.281	1.931	14.1
9	858.103	2.860	15.1	28	566.919	1.889	11.2
10	809.756	2.699	7.3	29	538.350	1.794	84.5
11	801.789	2.672	7.5	30	527.911	1.759	10.0
12	791.900	2.639	8.7	31	518.846	1.729	6.8
13	782.560	2.608	8.3	32	477.915	1.593	30.8
14	728.719	2.429	8.6	33	388.362	1.294	6.5
15	722.400	2.408	10.6	34	381.220	1.271	11.3
16	720.203	2.400	9.2	35	374.078	1.247	4.7
17	711.687	2.372	9.1	36	228.211	0.761	76.4
18	703.171	2.344	8.3	37	23.832	0.079	3.8
19	692.733	2.309	7.8	38	24.382	0.081	3.9
20	683.942	2.279	5.9	39	2.955	0.010	10.7



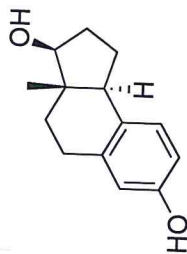
MQ 1030



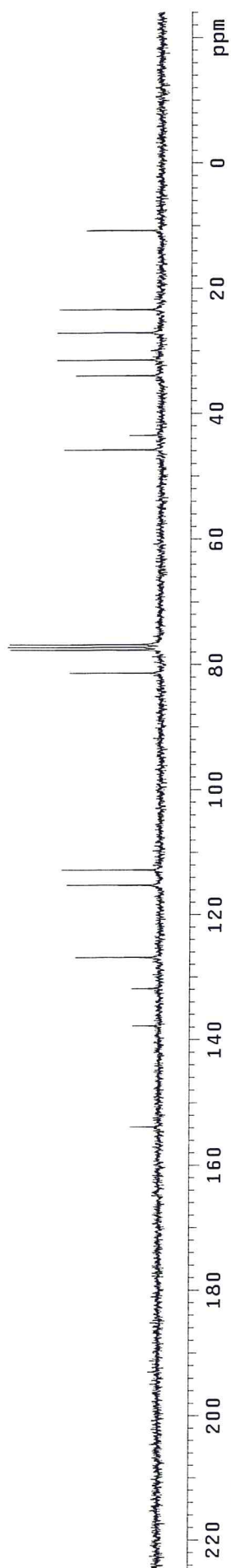
INDEX	FREQUENCY	PPM	HEIGHT
1	16999.250	221.338	5.6
2	11561.906	153.245	8.2
3	10155.607	134.606	8.4
4	10133.848	134.317	7.4
5	9758.224	129.339	6.9
6	9326.486	123.616	16.9
7	8811.148	116.786	17.4
8	5856.546	77.625	7.7
9	5824.480	77.200	8.5
10	5792.415	76.775	7.8
11	3639.449	48.238	8.4
12	3502.025	46.417	17.9
13	3081.739	40.846	55.1
14	2811.473	37.264	58.5
15	2771.391	36.733	23.1
16	2766.810	36.672	14.4
17	2207.955	29.265	66.0
18	2195.358	29.098	20.2
19	1951.432	25.865	17.3
20	1635.358	21.676	19.1
21	1043.292	13.828	19.5



INDEX	FREQUENCY	PPM	HEIGHT
1	11604.278	153.807	4.6
2	10394.952	137.778	4.2
3	9947.181	131.843	4.4
4	9566.977	126.804	13.8
5	8692.048	115.207	15.3
6	8506.526	112.748	16.1
7	6135.973	81.328	14.9
8	5857.691	77.640	24.5
9	5825.625	77.215	24.9
10	5793.560	76.790	24.6
11	3453.927	45.780	15.9
12	3278.712	43.457	5.1
13	2558.384	33.910	14.0
14	2369.427	31.405	17.1
15	2039.611	27.034	17.1
16	1761.329	23.345	16.8
17	808.527	10.716	12.4

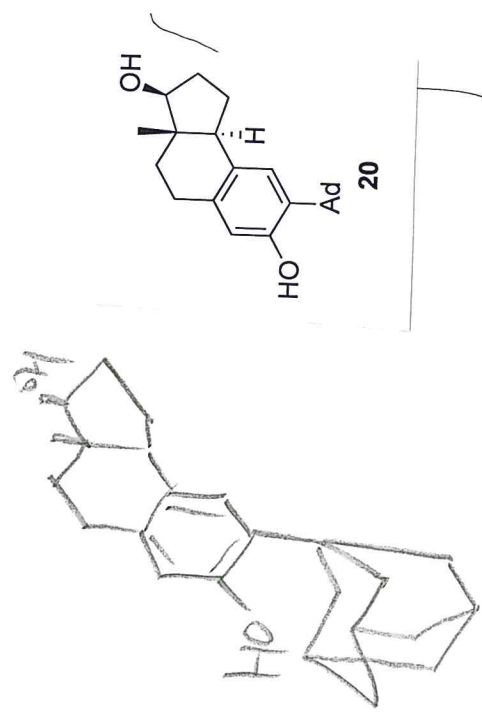


19

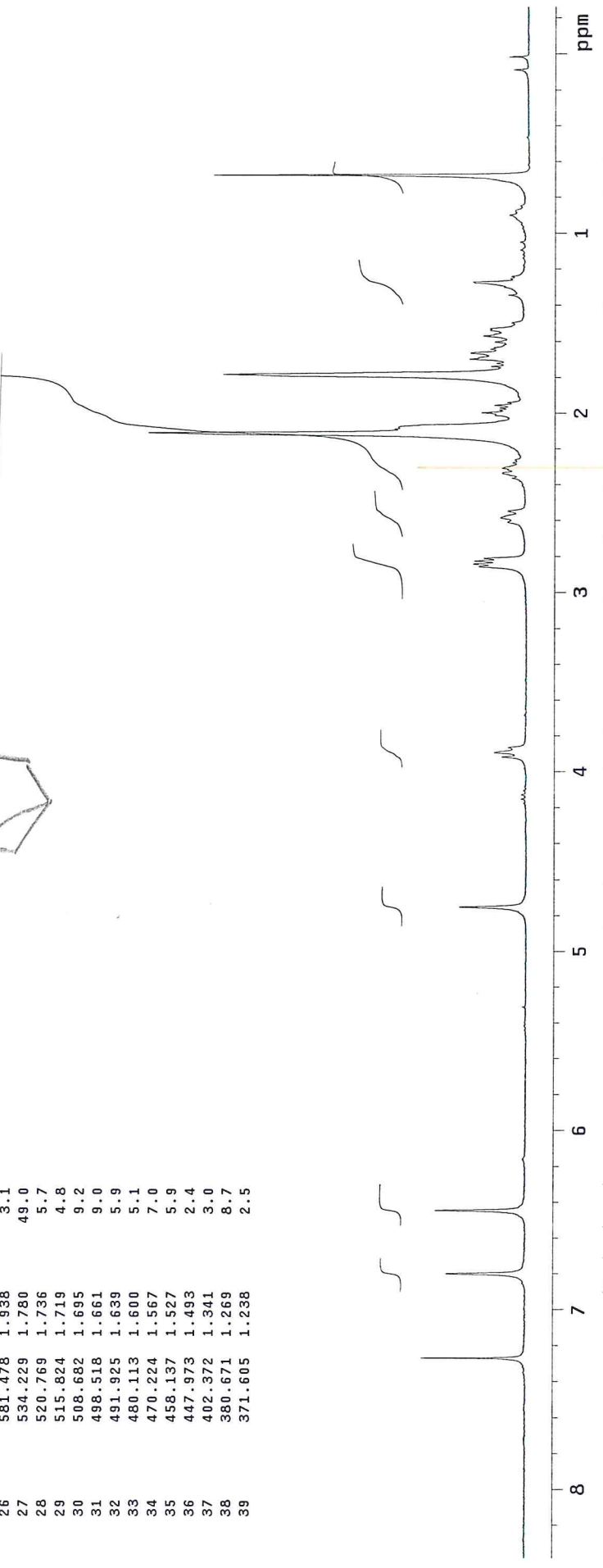


1031

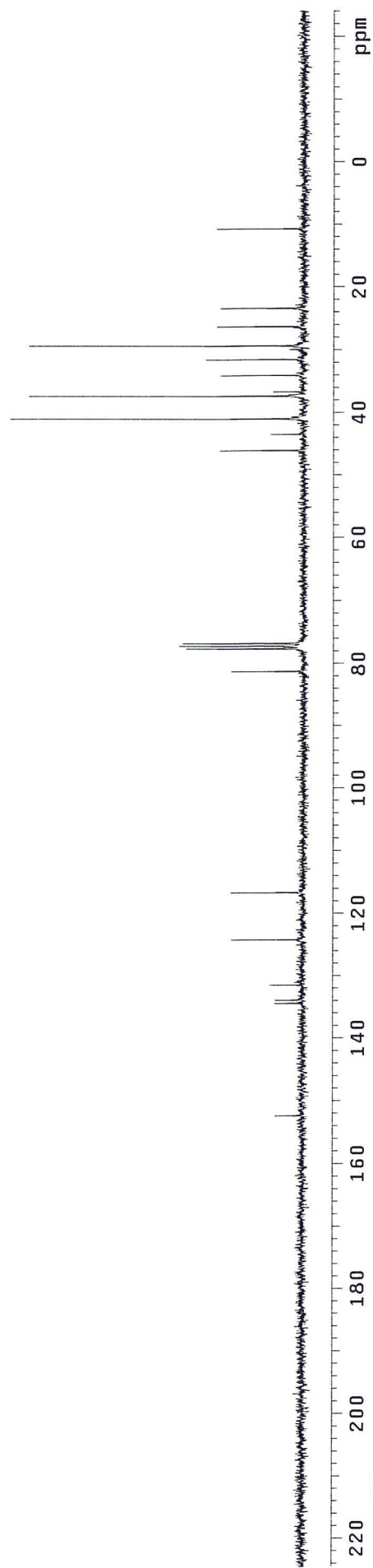
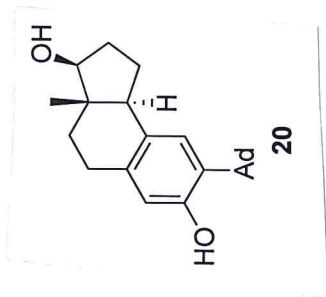
INDEX	FREQUENCY PPM	HEIGHT	INDEX	FREQUENCY PPM	HEIGHT
1	2181.345	7.270	40	269.141	0.897
2	2040.148	6.799	41	201.565	0.672
3	1933.838	6.445	42	25.480	0.085
4	1425.364	4.750	43	4.054	0.014
5	1174.835	3.915			
6	1167.693	3.892			
7	1158.628	3.861			
8	856.181	2.853			
9	852.060	2.840			
10	846.841	2.822			
11	842.445	2.808			
12	782.286	2.607			
13	774.594	2.582			
14	763.606	2.545			
15	708.665	2.362			
16	699.600	2.332			
17	691.634	2.305			
18	682.843	2.276			
19	678.448	2.261			
20	632.573	2.108			
21	626.529	2.088			
22	598.510	1.995			
23	594.114	1.980			
24	590.269	1.967			
25	586.148	1.954			
26	581.478	1.938			
27	534.229	1.780			
28	520.769	1.736			
29	515.824	1.719			
30	508.682	1.695			
31	498.518	1.661			
32	491.925	1.639			
33	480.113	1.600			
34	470.224	1.567			
35	458.137	1.527			
36	447.973	1.493			
37	402.372	1.341			
38	380.671	1.269			
39	371.605	1.238			



20



INDEX	FREQUENCY	PPM	HEIGHT
1	11497.775	152.395	4.4
2	10143.009	134.439	4.4
3	10104.073	133.923	4.3
4	9920.842	131.494	5.2
5	9371.148	124.208	11.7
6	8801.986	116.665	11.8
7	6131.392	81.268	11.8
8	5856.545	77.625	19.1
9	5824.480	77.200	20.4
10	5792.415	76.775	19.7
11	3474.540	46.053	13.7
12	3279.857	43.472	5.2
13	3092.045	40.983	47.5
14	2816.053	37.325	44.5
15	2764.520	36.642	4.8
16	2566.401	34.016	13.6
17	2376.298	31.496	16.0
18	2211.390	29.311	44.4
19	1983.497	26.290	14.2
20	1763.619	23.376	13.7
21	805.091	10.671	14.3

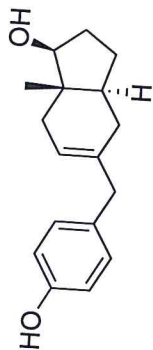


INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2481.533	8.270	1.4	40	362.204	1.207	12.1
2	2432.087	8.106	33.8	41	356.435	1.188	9.1
3	2079.643	6.931	32.8	42	350.941	1.170	8.8
4	2071.128	6.903	29.3	43	345.447	1.151	7.2
5	2007.397	6.690	41.3	44	336.656	1.122	4.4
6	2005.199	6.683	20.0	45	329.514	1.098	3.0
7	2000.804	6.668	19.7	46	245.730	0.819	5.9
8	1998.881	6.662	26.5	47	242.433	0.808	5.0
9	1977.729	6.591	1.8	48	181.449	0.605	100.0
10	1607.979	5.359	13.8	49	161.946	0.540	2.7
11	1110.218	3.700	12.9	50	117.993	0.393	1.3
12	1101.153	3.670	9.9				
13	1092.637	3.642	10.9				
14	932.486	3.108	40.5				
15	608.337	2.027	10.0				
16	604.217	2.014	10.8				
17	597.898	1.993	12.1				
18	595.701	1.985	14.5				
19	593.778	1.979	17.5				
20	591.580	1.972	16.8				
21	570.428	1.901	12.5				
22	567.681	1.892	15.9				
23	562.462	1.875	17.1				
24	558.341	1.861	18.2				
25	549.551	1.832	27.0				
26	539.936	1.799	14.0				
27	535.541	1.785	17.5				
28	466.591	1.555	15.9				
29	455.053	1.517	20.0				
30	449.559	1.498	23.7				
31	446.263	1.487	24.6				
32	439.395	1.464	21.6				
33	434.176	1.447	18.3				
34	429.780	1.432	16.4				
35	420.990	1.403	13.3				
36	417.144	1.390	11.9				
37	408.079	1.360	7.1				
38	404.233	1.347	6.2				
39	373.192	1.244	9.8				

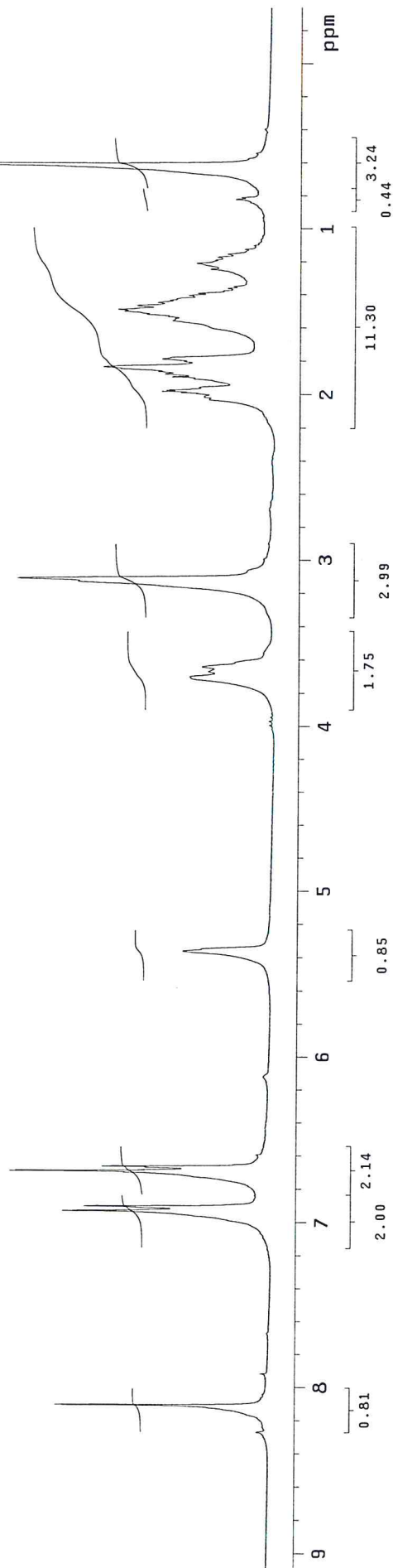
1129



in acetone-d₆

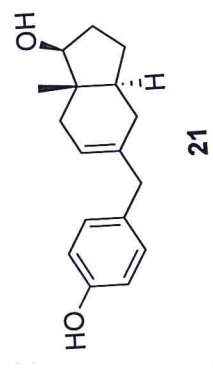


21

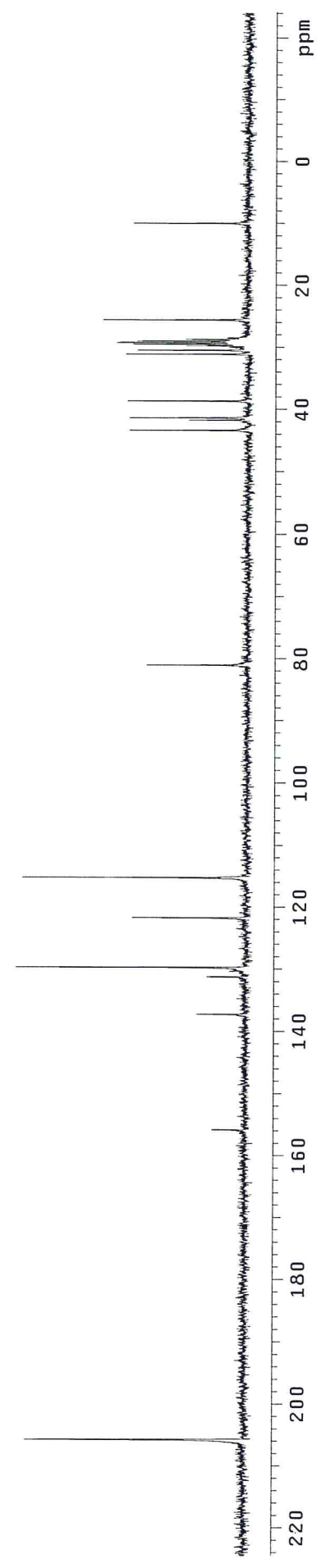


1129

INDEX	FREQUENCY	PPM	HEIGHT
1	15523.393	205.751	35.2
2	11753.412	155.783	5.3
3	10351.693	137.204	7.8
4	9898.196	131.193	6.2
5	9783.677	129.676	37.0
6	9180.159	121.676	18.2
7	8690.016	115.180	36.0
8	6109.892	80.982	16.1
9	3266.373	43.293	18.9
10	3142.692	41.654	9.4
11	3115.208	41.290	18.9
12	2911.363	38.588	19.3
13	2341.056	31.029	19.5
14	2292.958	30.391	17.7
15	2237.988	29.663	9.8
16	2218.520	29.405	18.5
17	2200.197	29.162	21.0
18	2180.729	28.904	17.8
19	2161.260	28.646	10.0
20	1924.205	25.504	23.2
21	748.090	9.915	18.4



21



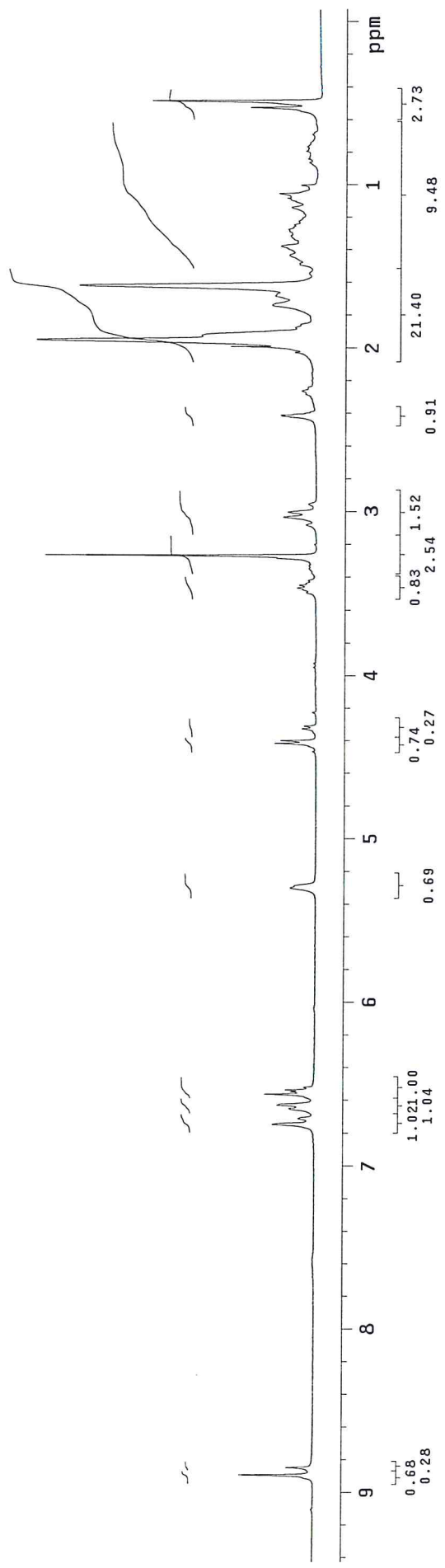
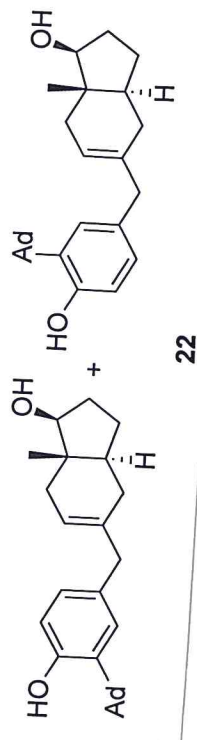
26

STANDARD 1H OBSERVE

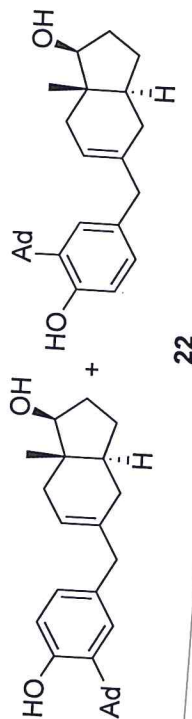
exp1 std1h

SAMPLE		DEC. & VT	
date	Sep 23 2008	dfrq	300.050
solvent	DMSO	dn	H1
file		dpwr	30
ACQUISITION		dof	0
sfrq	300.050	dm	nmn
tn	H1	dmm	c
at	1.998	dmc	200
np	17984	wtfile	PROCESSING
sw	4500.5	proc	ft
fb	2600	fn	not used
bs	16		
tpwr	49	werr	
pw	7.0	wexp	
dl	1.000	wbs	
tof	0	wnt	
nt	8		
ct	8		
alock	not used		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-23.3		
wp	2852.0		
vs	45		
sc	0		
wc	250		
hzmm	11.41		
fs	3075.20		
rfl	771.3		
rfp	0		
th	1		
ins	1.000		
nm	cdc		
ph			

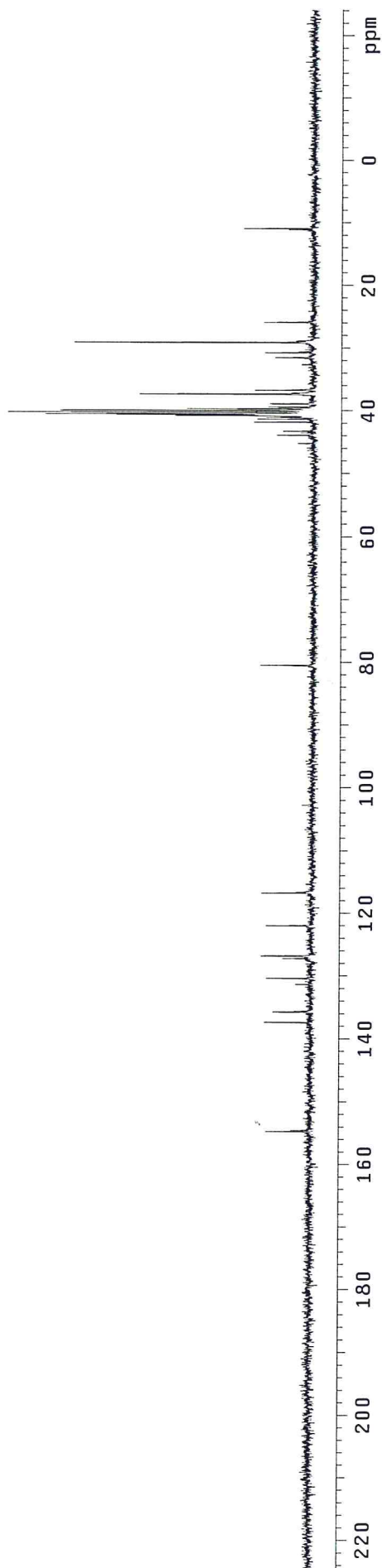
MQ 1130
C1177) in DMSO-d6



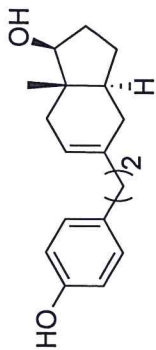
INDEX	FREQUENCY	PPM	HEIGHT
1	11672.100	154.705	7.1
2	11654.922	154.478	3.0
3	10363.142	137.356	7.4
4	10238.316	135.701	6.0
5	10226.864	135.550	2.6
6	9907.355	131.315	2.4
7	9835.207	130.359	7.1
8	9595.862	127.186	4.5
9	9568.377	126.822	8.0
10	9562.651	126.746	7.4
11	9200.769	121.950	7.2
12	8805.677	116.713	7.9
13	6067.517	80.421	8.2
14	3406.084	45.145	2.5
15	3308.742	43.855	5.7
16	3278.967	43.460	2.0
17	3258.354	43.187	4.7
18	3150.705	41.760	9.4
19	3114.059	41.275	8.9
20	3093.446	41.001	7.5
21	3072.832	40.728	22.0
22	3063.671	40.607	31.3
23	3052.219	40.455	42.7
24	3031.605	40.182	48.6
25	3010.992	39.909	40.3
26	2989.233	39.620	20.1
27	2968.619	39.347	7.1
28	2929.683	38.831	6.9
29	2814.018	37.298	27.6
30	2767.065	36.675	9.3
31	2456.717	32.562	1.8
32	2373.118	31.454	6.1
33	2314.713	30.680	7.7
34	2192.177	29.056	38.0
35	1949.396	25.838	7.8
36	833.976	11.054	4.0
37	820.234	10.872	11.1



22

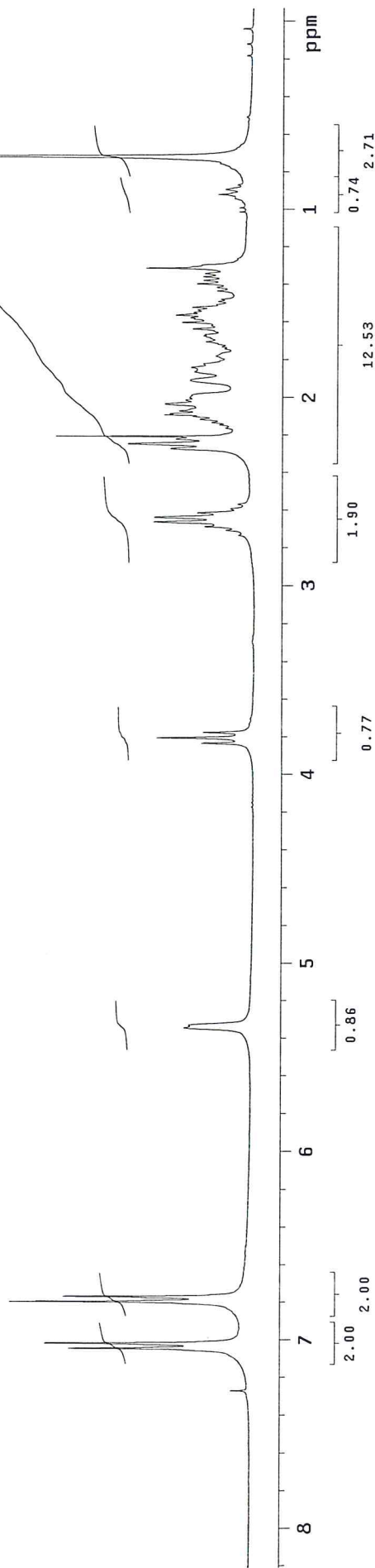


1151



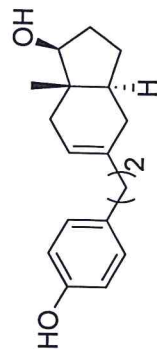
23

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2181.345	7.270	3.2	40	518.571	1.728	5.3
2	2114.043	7.046	29.2	41	510.880	1.703	7.7
3	2105.802	7.018	33.0	42	501.540	1.672	8.2
4	2039.324	6.797	38.6	43	499.617	1.665	8.0
5	2031.083	6.769	30.1	44	490.552	1.635	9.8
6	1603.371	5.344	10.9	45	485.607	1.618	7.0
7	1599.800	5.332	10.2	46	480.113	1.600	11.6
8	1149.837	3.832	8.3	47	474.894	1.583	9.7
9	1141.322	3.804	15.5	48	472.696	1.575	10.3
10	1132.531	3.775	8.0	49	468.575	1.562	12.6
11	819.370	2.731	2.5	50	464.730	1.549	9.8
12	811.404	2.704	4.4	51	460.334	1.534	9.2
13	805.635	2.685	7.9	52	456.214	1.520	10.0
14	798.218	2.660	16.1	53	452.093	1.507	6.2
15	790.801	2.636	16.0	54	446.874	1.489	5.8
16	783.934	2.613	9.1	55	443.578	1.478	5.4
17	777.341	2.591	3.8	56	430.117	1.433	6.0
18	770.199	2.567	2.6	57	424.623	1.415	6.1
19	681.195	2.270	13.4	58	418.580	1.395	9.2
20	673.503	2.245	20.2	59	413.360	1.378	8.2
21	665.537	2.218	12.5	60	407.317	1.358	8.3
22	661.417	2.204	31.7	61	402.372	1.341	7.9
23	648.231	2.160	4.6	62	393.582	1.312	17.4
24	643.286	2.144	5.5	63	377.924	1.260	2.8
25	639.166	2.130	6.8	64	303.205	1.011	2.5
26	634.221	2.114	8.7	65	296.612	0.989	2.4
27	629.826	2.099	9.8	66	275.460	0.918	5.9
28	627.079	2.090	14.4	67	267.219	0.891	4.7
29	624.881	2.083	13.5	68	260.076	0.867	2.8
30	620.761	2.069	12.0	69	225.738	0.752	5.6
31	609.772	2.032	14.3	70	214.750	0.716	101.0
32	603.729	2.012	11.0	71	11.196	0.037	1.9
33	599.883	1.999	10.3				
34	572.413	1.908	10.2				
35	558.678	1.862	9.6				
36	551.810	1.839	10.1				
37	546.042	1.820	8.2				
38	533.680	1.779	6.2				
39	521.868	1.739	4.8				

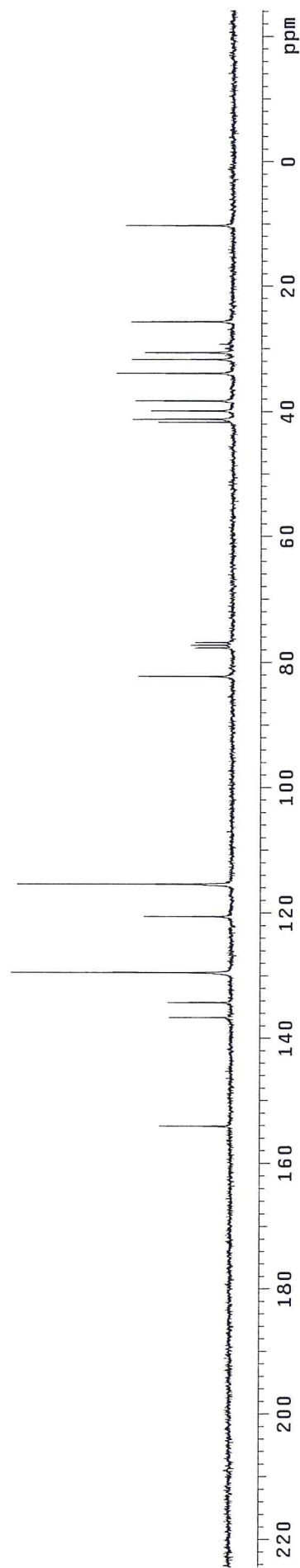


1151

INDEX	FREQUENCY	PPM	HEIGHT
1	11622.602	154.050	11.4
2	10307.918	136.625	9.9
3	10126.977	134.226	10.1
4	9765.096	129.430	35.2
5	9091.721	120.505	14.0
6	8703.500	115.359	34.2
7	6196.669	82.133	14.9
8	5857.691	77.640	5.9
9	5825.626	77.215	6.6
10	5793.560	76.790	5.8
11	3138.999	41.605	11.9
12	3104.643	41.150	16.0
13	3003.866	39.814	13.0
14	2883.620	38.220	15.5
15	2553.804	33.849	18.6
16	2386.606	31.633	16.1
17	2305.297	30.555	14.0
18	1934.254	25.637	16.2
19	768.446	10.185	17.1

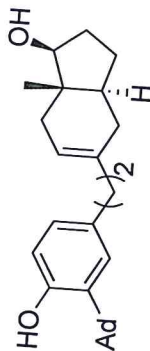


23

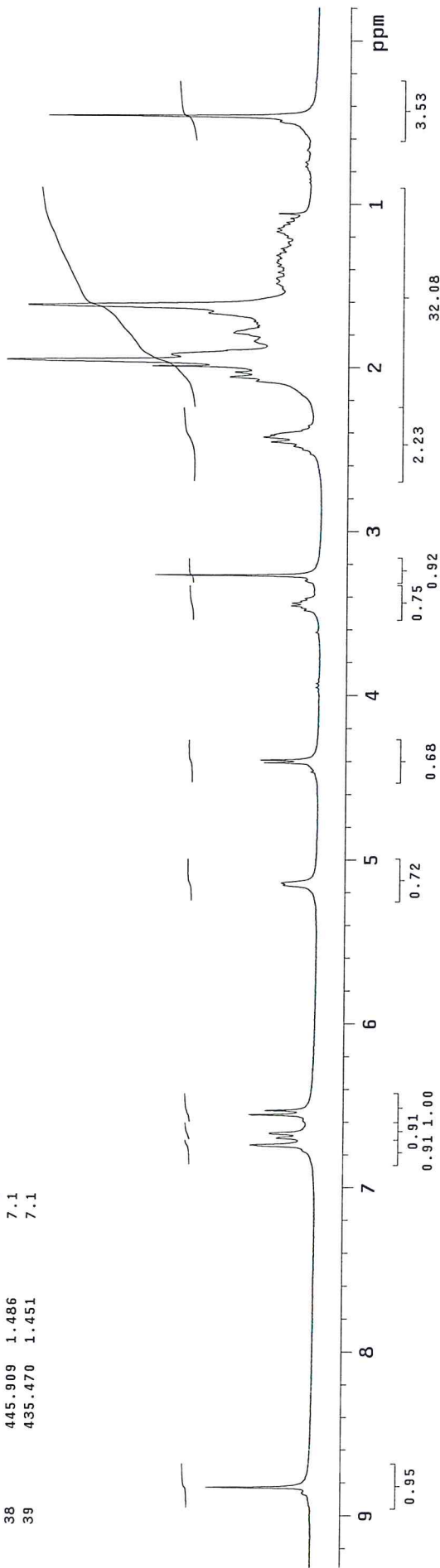


1153

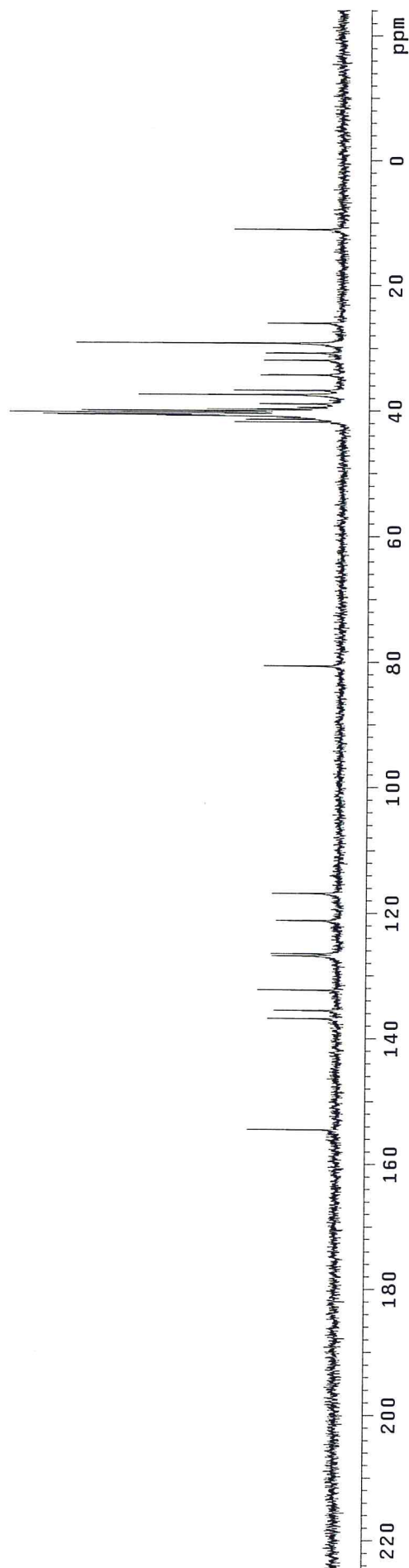
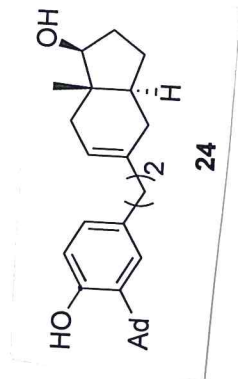
INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2659.187	8.863	1.5	40	424.482	1.415	6.9
2	2649.572	8.830	16.9	41	413.769	1.379	6.9
3	2022.426	6.740	10.3	42	406.077	1.353	7.1
4	2009.515	6.697	6.0	43	401.957	1.340	7.0
5	2000.176	6.666	7.2	44	393.441	1.311	7.2
6	1966.937	6.555	10.5	45	385.200	1.284	6.1
7	1958.970	6.529	7.9	46	381.079	1.270	6.5
8	1546.642	5.155	5.3	47	368.992	1.230	5.3
9	1542.796	5.142	5.6	48	349.489	1.165	7.1
10	1338.692	4.462	1.0	49	344.544	1.148	7.0
11	1322.210	4.407	8.5	50	332.182	1.107	5.6
12	1317.540	4.391	9.1	51	332.732	1.109	5.6
13	1125.798	3.752	-0.5	52	325.040	1.083	5.0
14	1043.936	3.479	2.3	53	316.799	1.056	6.8
15	1035.695	3.452	4.4	54	259.112	0.864	1.9
16	1030.751	3.435	4.2	55	253.068	0.843	2.0
17	1022.235	3.407	2.2	56	230.268	0.767	2.6
18	989.545	3.298	2.1	57	222.301	0.741	2.6
19	980.205	3.267	26.1	58	200.050	0.667	2.4
20	867.028	2.890	-0.7	59	147.582	0.492	6.8
21	743.687	2.479	4.1	60	138.242	0.461	43.6
22	735.995	2.453	7.8				
23	727.479	2.425	8.9				
24	723.359	2.411	7.9				
25	721.710	2.405	7.2				
26	624.740	2.082	10.3				
27	617.598	2.058	14.4				
28	608.258	2.027	13.6				
29	597.820	1.992	26.8				
30	587.106	1.957	50.0				
31	575.843	1.919	23.8				
32	550.846	1.836	10.6				
33	536.561	1.788	13.9				
34	524.199	1.747	10.1				
35	515.134	1.717	10.6				
36	499.751	1.666	17.9				
37	486.290	1.621	46.6				
38	445.909	1.486	7.1				
39	435.470	1.451	7.1				



24

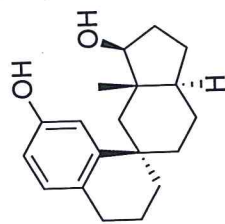


INDEX	FREQUENCY	PPM	HEIGHT
1	11653.777	154.462	14.2
2	10320.770	136.794	11.1
3	10223.428	135.504	10.0
4	9978.357	132.256	12.6
5	9564.941	126.776	10.4
6	9538.602	126.427	10.6
7	9138.929	121.130	9.8
8	8810.258	116.774	10.4
9	6077.823	80.557	12.0
10	3144.979	41.684	17.0
11	3115.204	41.290	15.1
12	3093.446	41.001	10.3
13	3072.832	40.728	29.4
14	3061.380	40.576	45.2
15	3052.219	40.455	47.6
16	3031.605	40.182	53.0
17	3009.846	39.893	41.4
18	2989.233	39.620	21.4
19	2968.619	39.347	6.9
20	2927.392	38.800	12.9
21	2817.454	37.343	32.3
22	2764.775	36.645	17.1
23	2578.108	34.171	12.8
24	2400.603	31.818	12.3
25	2314.713	30.680	12.0
26	2195.613	29.101	42.3
27	1955.122	25.914	11.7
28	825.960	10.948	17.2

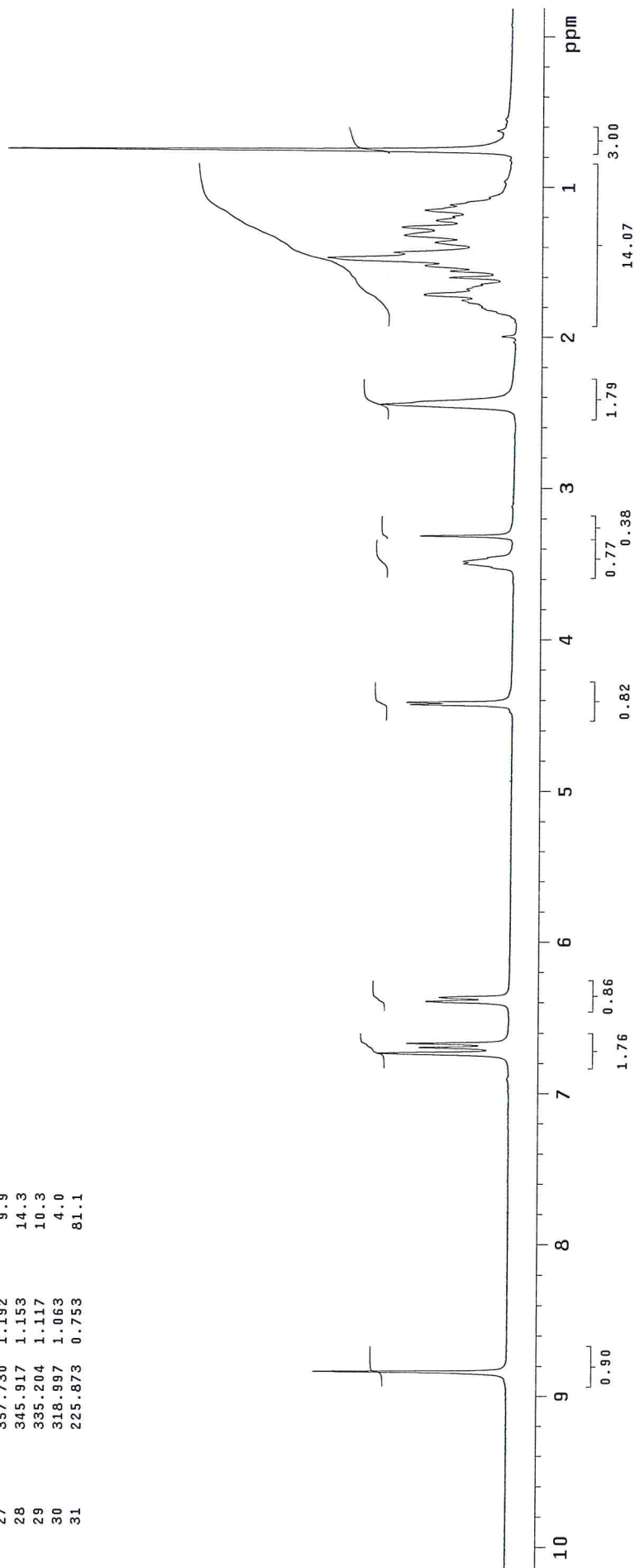


1169

INDEX	FREQUENCY	PPM	HEIGHT
1	2652.044	8.839	31.1
2	2020.504	6.734	21.2
3	2008.966	6.695	14.4
4	2001.000	6.669	16.4
5	1917.765	6.392	13.4
6	1909.798	6.365	11.3
7	1328.253	4.427	16.3
8	1324.133	4.413	16.8
9	1048.881	3.496	7.8
10	1043.936	3.479	7.9
11	993.941	3.313	14.8
12	733.797	2.446	21.1
13	525.298	1.751	8.3
14	515.134	1.717	14.3
15	514.310	1.714	14.4
16	503.047	1.677	7.6
17	493.433	1.645	5.3
18	480.247	1.601	10.4
19	467.061	1.557	10.2
20	456.348	1.521	14.3
21	441.239	1.471	29.8
22	430.251	1.434	19.2
23	409.923	1.366	12.6
24	395.639	1.319	17.6
25	379.156	1.264	18.0
26	366.795	1.222	12.5
27	357.730	1.192	9.9
28	345.917	1.153	14.3
29	335.204	1.117	10.3
30	318.997	1.063	4.0
31	225.873	0.753	81.1

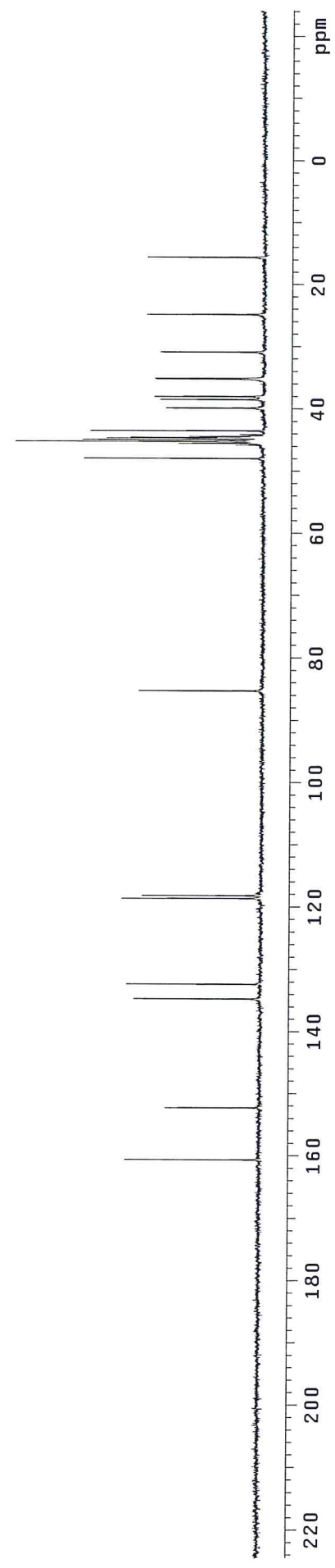
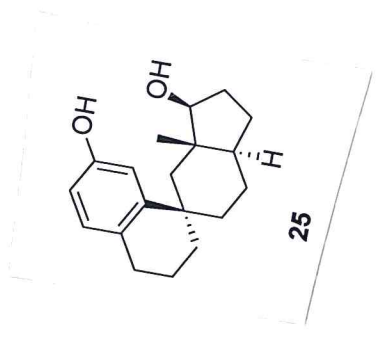


25

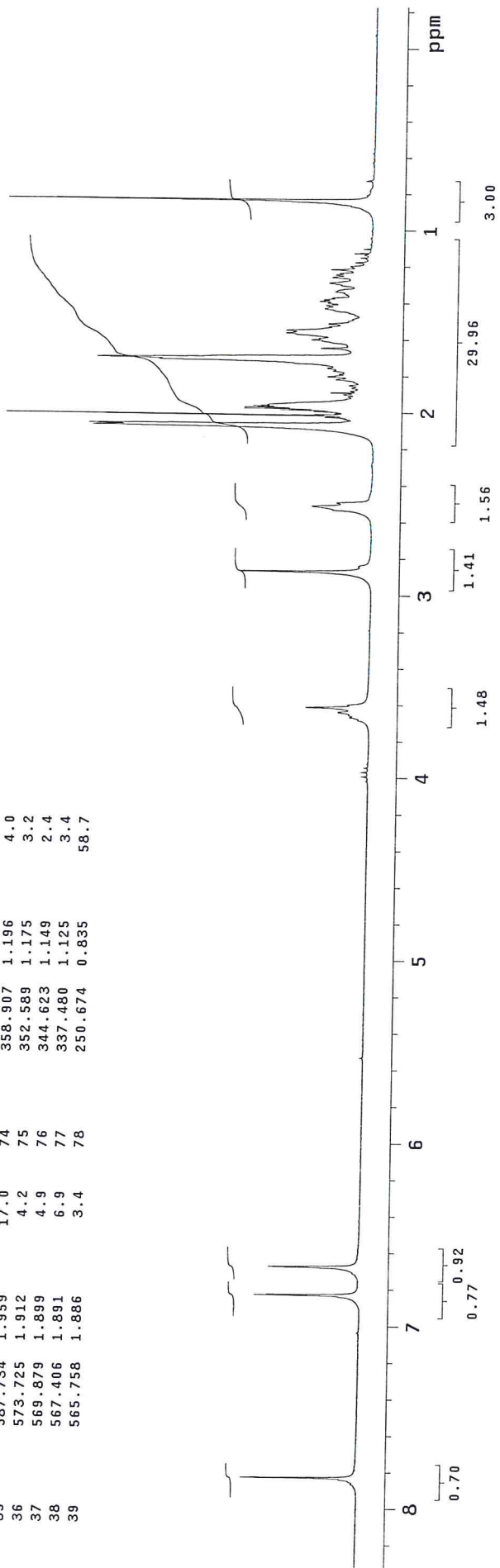
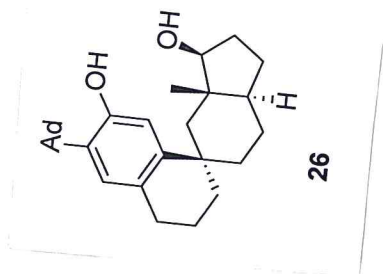
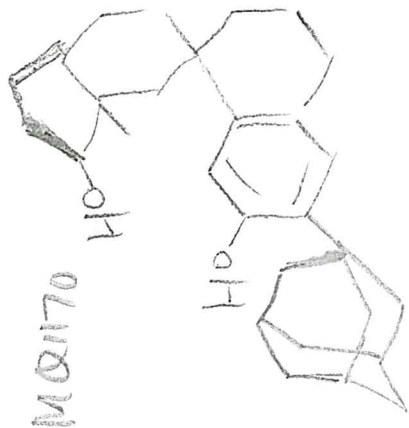


1169

INDEX	FREQUENCY	PPM	HEIGHT
1	12119.843	160.641	21.7
2	11488.841	152.277	15.2
3	10162.705	134.700	20.5
4	9984.055	132.332	21.6
5	8948.799	118.610	22.5
6	8915.588	118.170	19.2
7	6430.516	85.232	19.8
8	3613.336	47.892	28.9
9	3430.105	45.464	13.6
10	3409.492	45.191	39.9
11	3387.733	44.902	29.2
12	3367.120	44.629	25.3
13	3357.958	44.508	21.3
14	3346.506	44.356	11.9
15	3277.794	43.445	27.9
16	3002.948	39.802	15.7
17	2901.025	38.451	16.6
18	2864.379	37.965	17.6
19	2653.663	35.173	17.3
20	2646.792	35.081	17.5
21	2326.137	30.831	16.6
22	1869.205	24.775	18.8
23	1171.781	15.531	18.7



INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2350.225	7.833	18.5	40	564.659	1.892	3.8	4			
2	2049.701	6.831	16.8	41	559.165	1.864	3.5	5			
3	2003.551	6.677	14.6	42	555.045	1.850	3.9	6			
4	1100.329	3.667	3.0	43	545.156	1.817	6.0	7			
5	1092.088	3.640	4.9	44	540.760	1.802	7.4	8			
6	1084.122	3.613	10.1	45	536.640	1.789	5.6	9			
7	1079.726	3.598	3.4	46	531.146	1.770	6.5	10			
8	861.063	2.870	21.0	47	526.750	1.756	7.5	11			
9	753.929	2.513	9.5	48	514.114	1.713	34.3	12			
10	748.161	2.493	5.6	49	511.367	1.704	44.2	13			
11	623.171	2.077	44.6	50	494.061	1.647	8.6	14			
12	620.424	2.068	45.3	51	489.666	1.632	4.4	15			
13	613.007	2.043	3.9	52	480.326	1.601	10.1	16			
14	612.458	2.041	4.0	53	478.128	1.593	8.9	17			
15	610.535	2.035	4.6	54	469.338	1.564	14.1	18			
16	609.985	2.033	4.8	55	467.140	1.557	12.9	19			
17	609.436	2.031	5.0	56	464.942	1.550	14.1	20			
18	608.062	2.027	7.8	57	458.624	1.528	7.3	21			
19	607.513	2.025	7.6	58	453.954	1.513	7.4	22			
20	606.964	2.023	7.4	59	446.263	1.487	3.6	23			
21	606.414	2.021	7.3	60	429.231	1.431	8.0	24			
22	604.766	2.016	58.6	61	423.462	1.411	7.7	25			
23	604.217	2.014	13.0	62	419.616	1.398	7.6	26			
24	603.667	2.012	9.4	63	417.144	1.390	8.8	27			
25	603.118	2.010	6.5	64	414.397	1.381	8.1	28			
26	602.294	2.007	5.8	65	411.375	1.371	6.9	29			
27	601.744	2.005	6.3	66	406.705	1.355	4.7	30			
28	601.195	2.004	6.1	67	403.409	1.344	5.0	31			
29	600.645	2.002	5.8	68	401.211	1.337	6.3	32			
30	598.448	1.994	9.5	69	386.927	1.290	7.4	33			
31	596.250	1.987	14.9	70	377.312	1.258	6.8	34			
32	594.053	1.980	20.6	71	373.192	1.244	6.3	35			
33	591.855	1.973	20.6	72	370.719	1.236	5.7	36			
34	589.657	1.965	19.2	73	364.401	1.214	7.1	37			
35	587.734	1.959	17.0	74	358.907	1.196	4.0	38			
36	573.725	1.912	4.2	75	352.589	1.175	3.2	39			
37	569.879	1.899	4.9	76	344.623	1.149	2.4				
38	567.406	1.891	6.9	77	337.480	1.125	3.4				
39	565.758	1.886	3.4	78	250.674	0.835	58.7				



INDEX	FREQUENCY	PPM	HEIGHT
1	15501.634	205.463	61.5
2	11628.586	154.128	5.9
3	9625.640	127.581	6.0
4	9559.219	126.700	9.7
5	8663.676	114.831	9.2
6	6107.602	80.952	9.8
7	3248.050	43.051	8.6
8	3064.819	40.622	32.5
9	3030.463	40.167	10.0
10	3005.269	39.833	11.8
11	2870.136	38.042	6.8
12	2804.860	37.176	30.5
13	2732.713	36.220	6.5
14	2623.919	34.778	10.5
15	2527.723	33.503	9.8
16	2504.819	33.200	11.5
17	2290.667	30.361	10.0
18	2275.780	30.164	8.4
19	2252.876	29.860	6.9
20	2233.408	29.602	17.2
21	2213.939	29.344	40.5
22	2211.649	29.314	40.9
23	2195.616	29.101	43.4
24	2176.148	28.843	40.0
25	2156.680	28.585	22.6
26	2137.211	28.327	8.8
27	1945.964	25.792	10.4
28	1510.790	20.024	10.7
29	737.783	9.779	11.7

