

Synthesis of Hexacyclic Parnafungin A and C Models

Quan Zhou and Barry B. Snider*

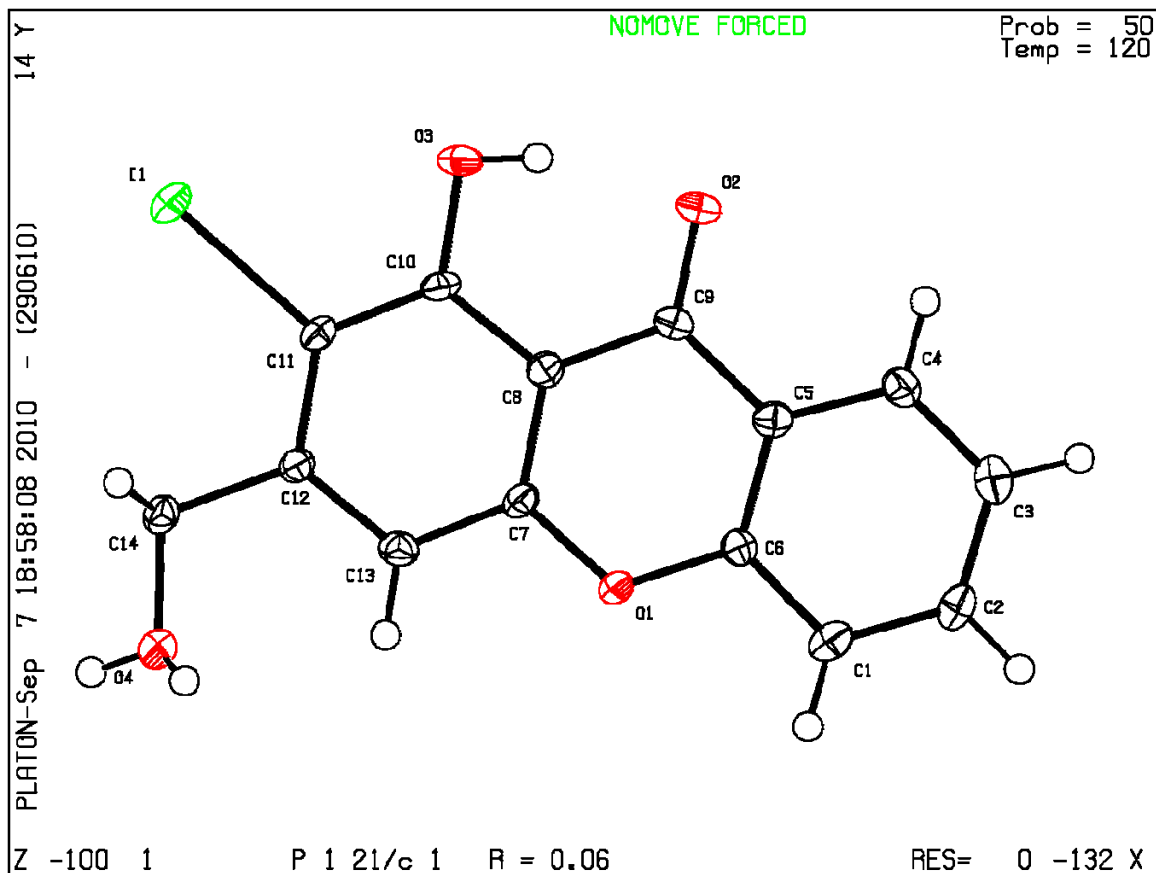
Department of Chemistry MS 015, Brandeis University,

Waltham, Massachusetts 02454-9110

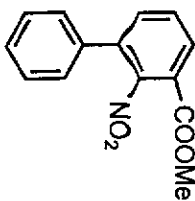
snider@brandeis.edu

X-ray Crystal Structure of **30a**.....S2

Copies of ^1H and ^{13}C NMR spectraS3-S47

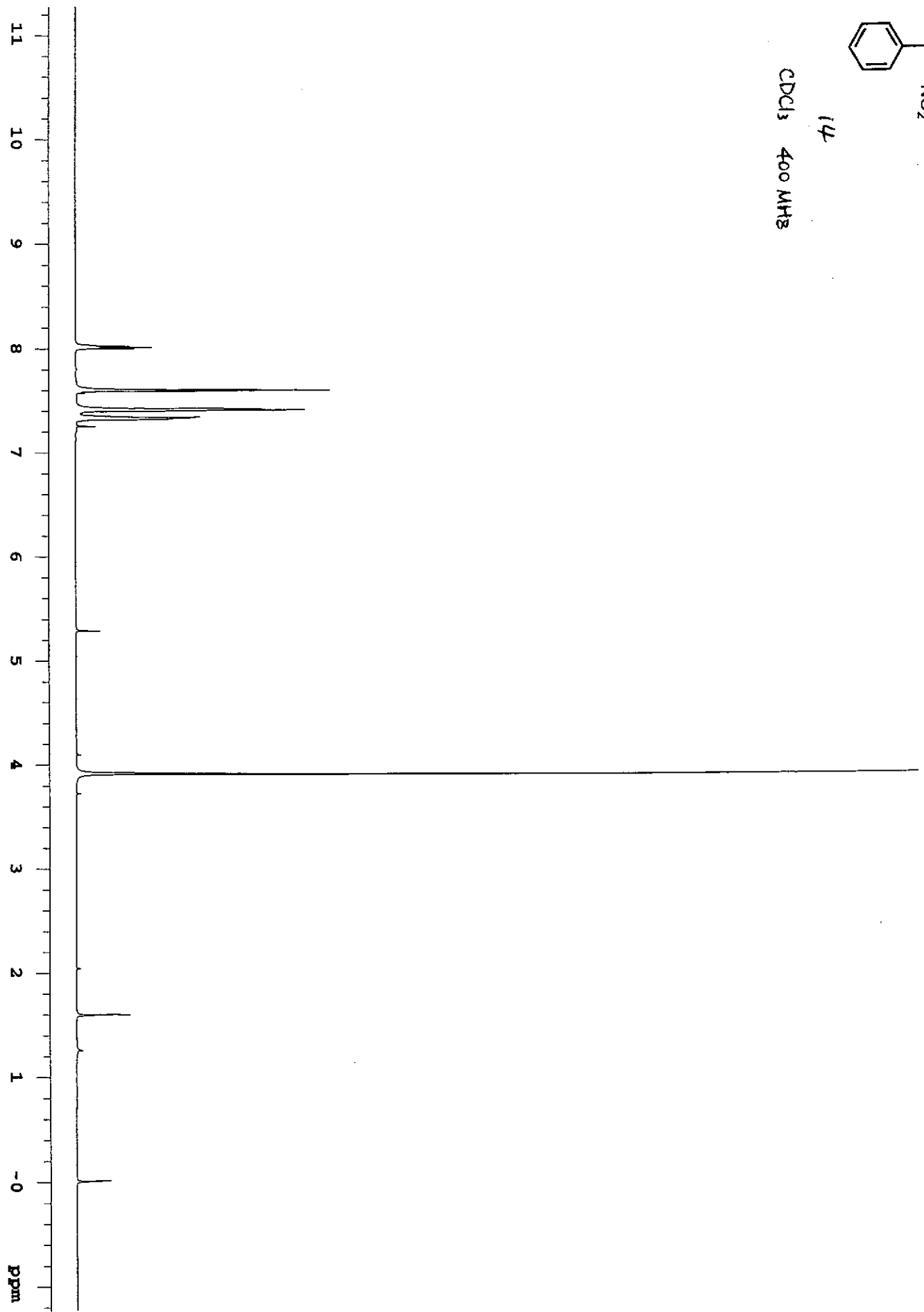
Figure S1. X-ray Crystal Structure of **30a**

S3



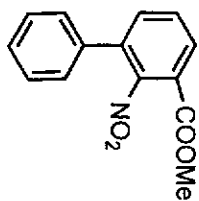
14

CDCl₃ 400 MHz

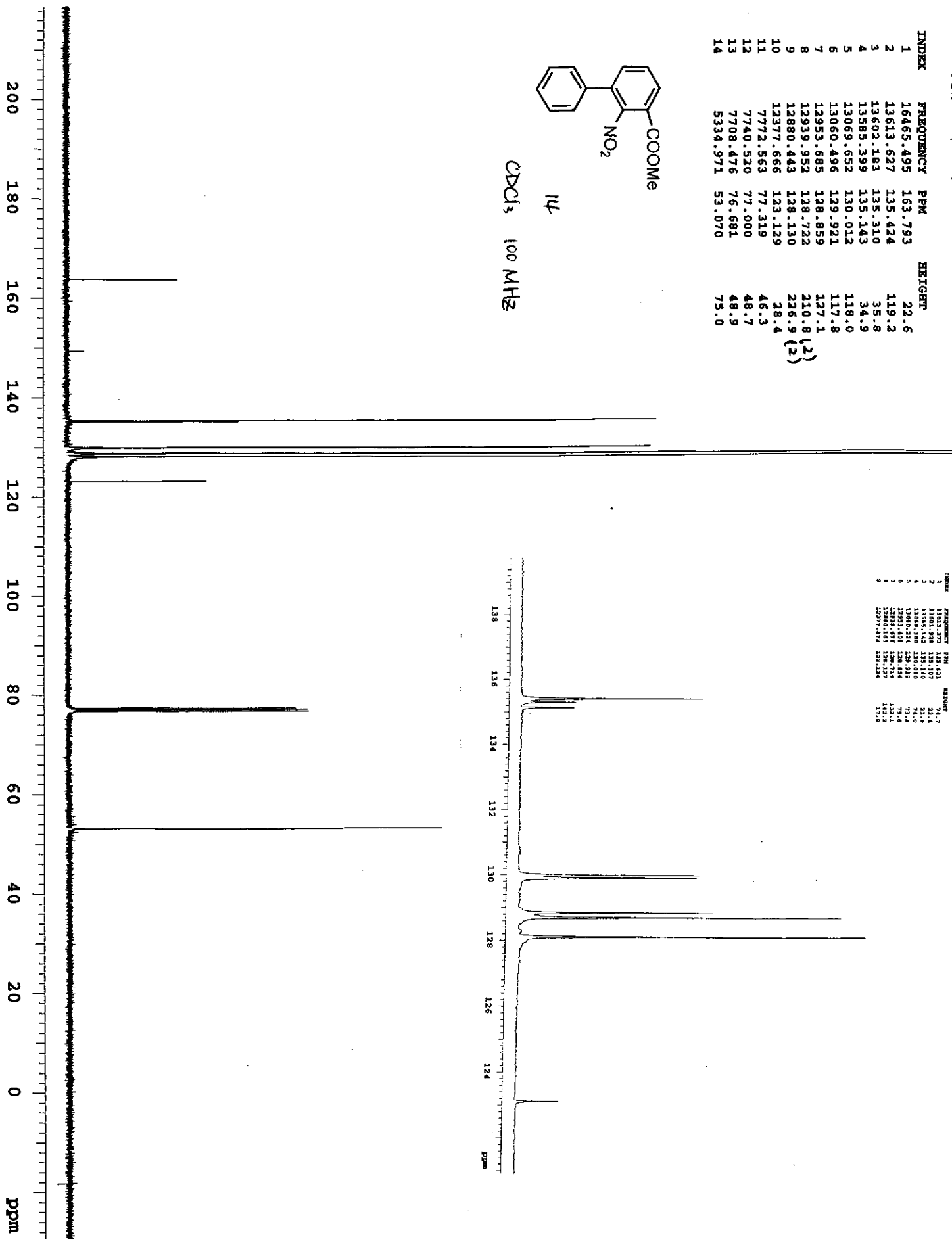


Scan - 4 - 23 - 3 - carbon

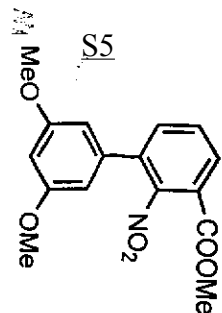
INDEX	FREQUENCY	PPM	HEIGHT
1	16465.495	163.793	22.6
2	13613.627	135.424	119.2
3	13602.183	135.310	35.8
4	13585.399	135.143	34.9
5	13069.652	130.012	118.0
6	13060.496	129.921	117.8
7	12953.685	128.859	127.1
8	12939.952	128.722	210.8 (2)
9	12880.443	128.130	226.9 (2)
10	12377.666	123.129	28.4
11	7772.563	77.319	46.3
12	7740.520	77.000	48.7
13	7708.476	76.681	48.9
14	5334.971	53.070	75.0



CDCl₃ 100 MHz

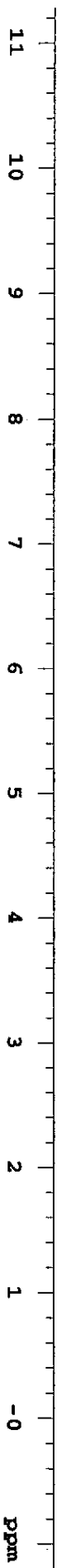


4 (Zhou-4-18-2

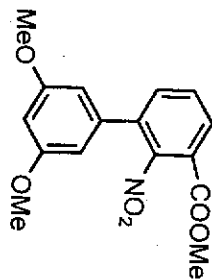


20b

CDCl₃ 400 MHz

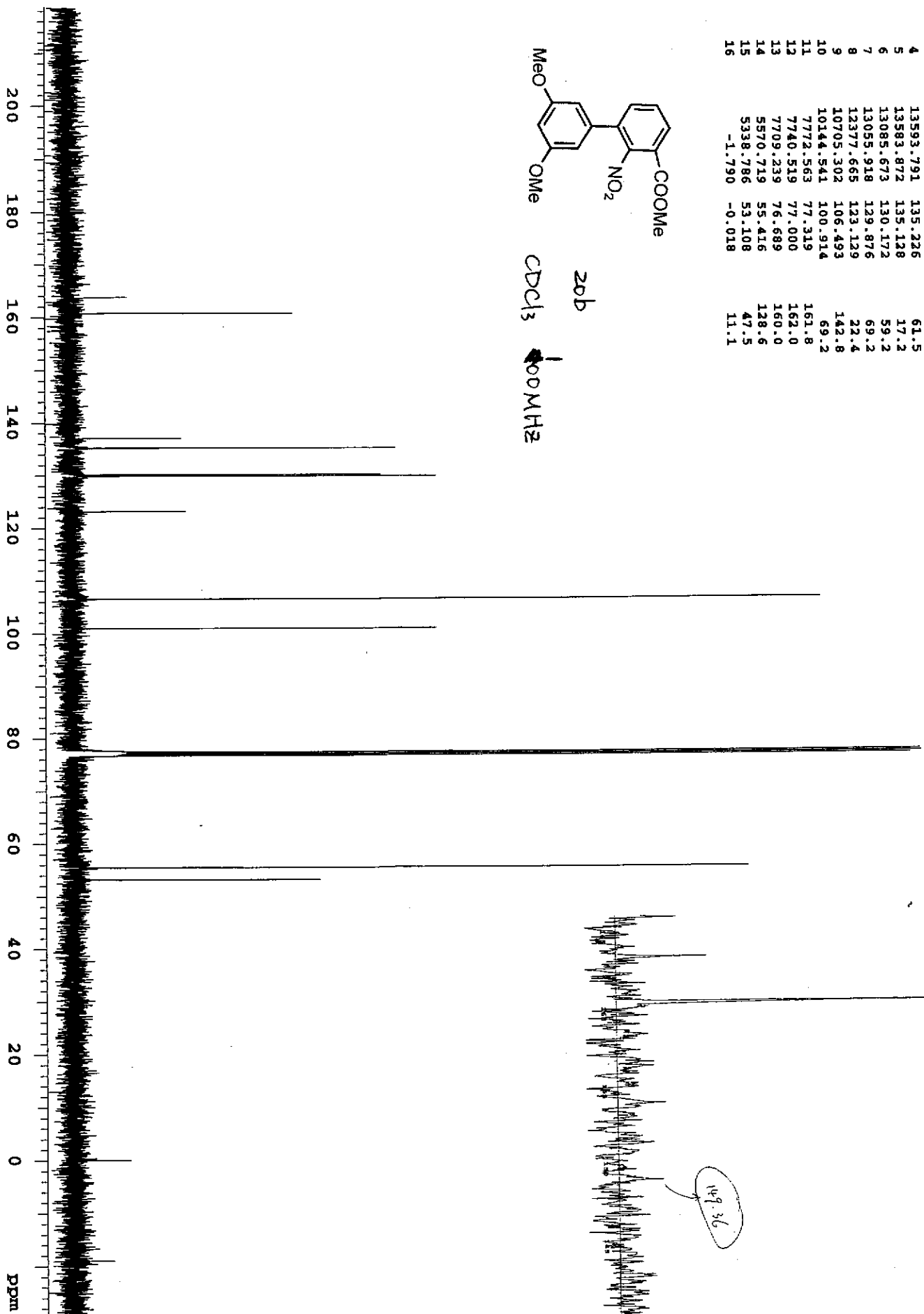


INDEX	FREQUENCY	PPM	HEIGHT
1	16463.969	163.778	11.0
2	16163.371	160.788	43.0
3	13780.711	137.086	21.6
4	13593.791	135.226	61.5
5	13583.872	135.128	17.2
6	13085.673	130.172	59.2
7	13055.918	129.876	69.2
8	12377.665	123.129	22.4
9	10705.302	106.493	142.8
10	10144.541	100.914	69.2
11	7772.563	77.319	161.8
12	7740.519	77.000	162.0
13	7709.239	76.689	160.0
14	5570.719	55.416	128.6
15	5338.786	53.108	47.5
16	-1.790	-0.018	11.1



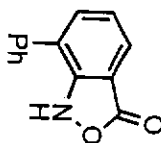
20b

CDCl₃ 100MHz



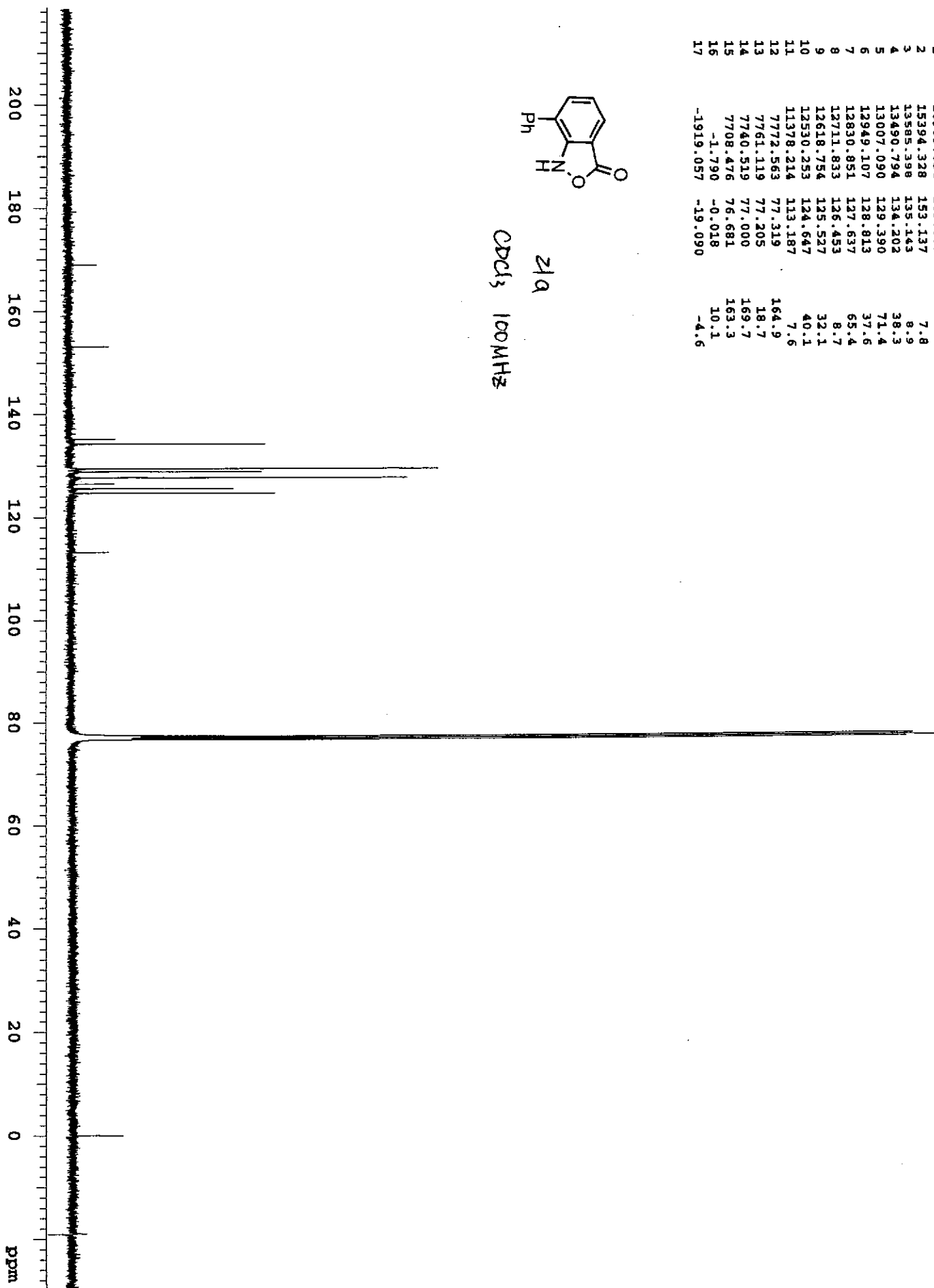
NAME: 20b
 EXPNO: 1
 F2: 100.628150
 F3: 100.628150
 PROCNO: 1
 GPC: 0
 HETERO: 0
 INSTRUM: spect
 NS: 1024
 NS2: 1024
 NS3: 1024
 SFO: 100.628150
 TD: 1024
 TD0: 1024
 TD1: 1024
 TD2: 1024
 TD3: 1024
 TE: 300.2
 URG: 0
 VER: 3.1

INDEX	FREQUENCY	PPM	HEIGHT
1	16989.634	169.007	5.3
2	15394.328	153.137	7.8
3	13585.398	135.143	8.9
4	13490.794	134.202	38.3
5	13007.090	129.390	71.4
6	12949.107	128.813	37.6
7	12830.851	127.637	65.4
8	12711.833	126.453	8.7
9	12618.754	125.527	32.1
10	12530.253	124.647	40.1
11	11378.214	113.187	7.6
12	7772.563	77.319	164.9
13	7761.119	77.205	18.7
14	7740.519	77.000	169.7
15	7708.476	76.681	163.3
16	-1.790	-0.018	10.1
17	-1919.057	-19.090	-4.6

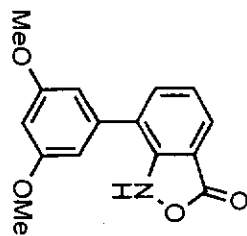


Z/A

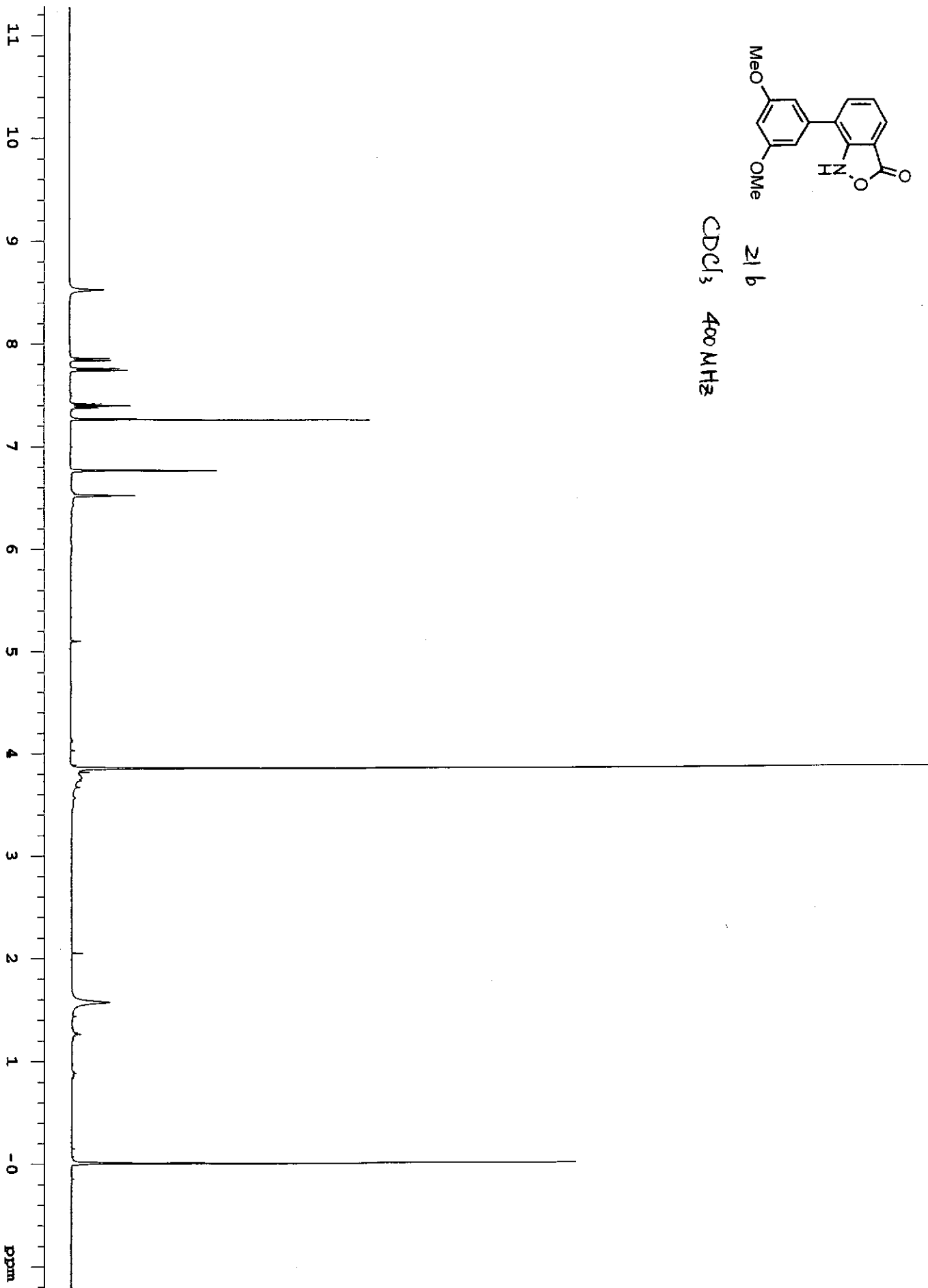
CDCl₃ 100MHz



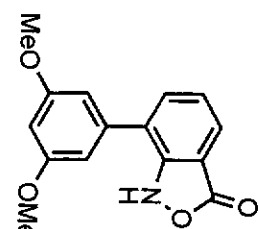
Qcom-4-31-1



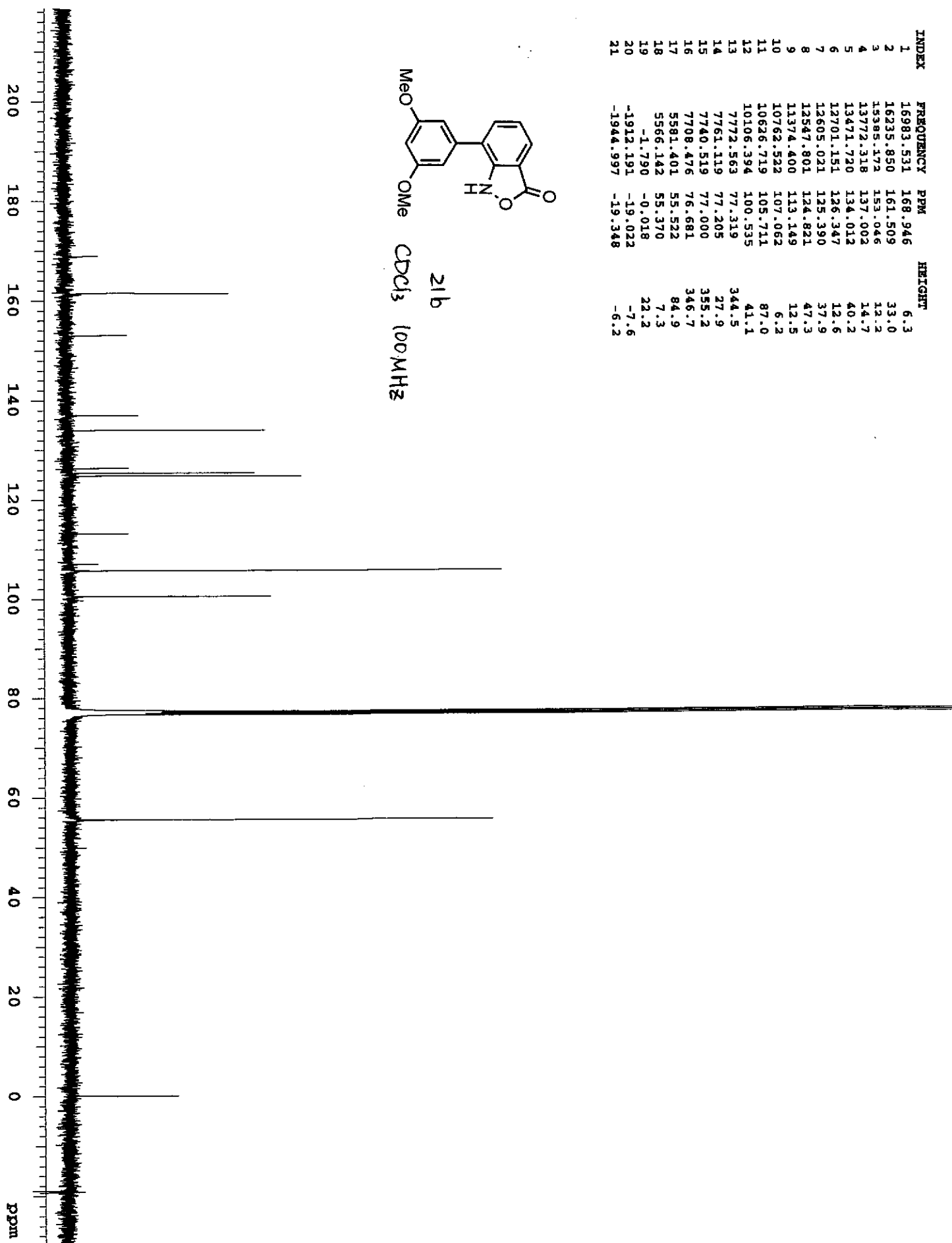
CDCl₃ 400 MHz
21 b

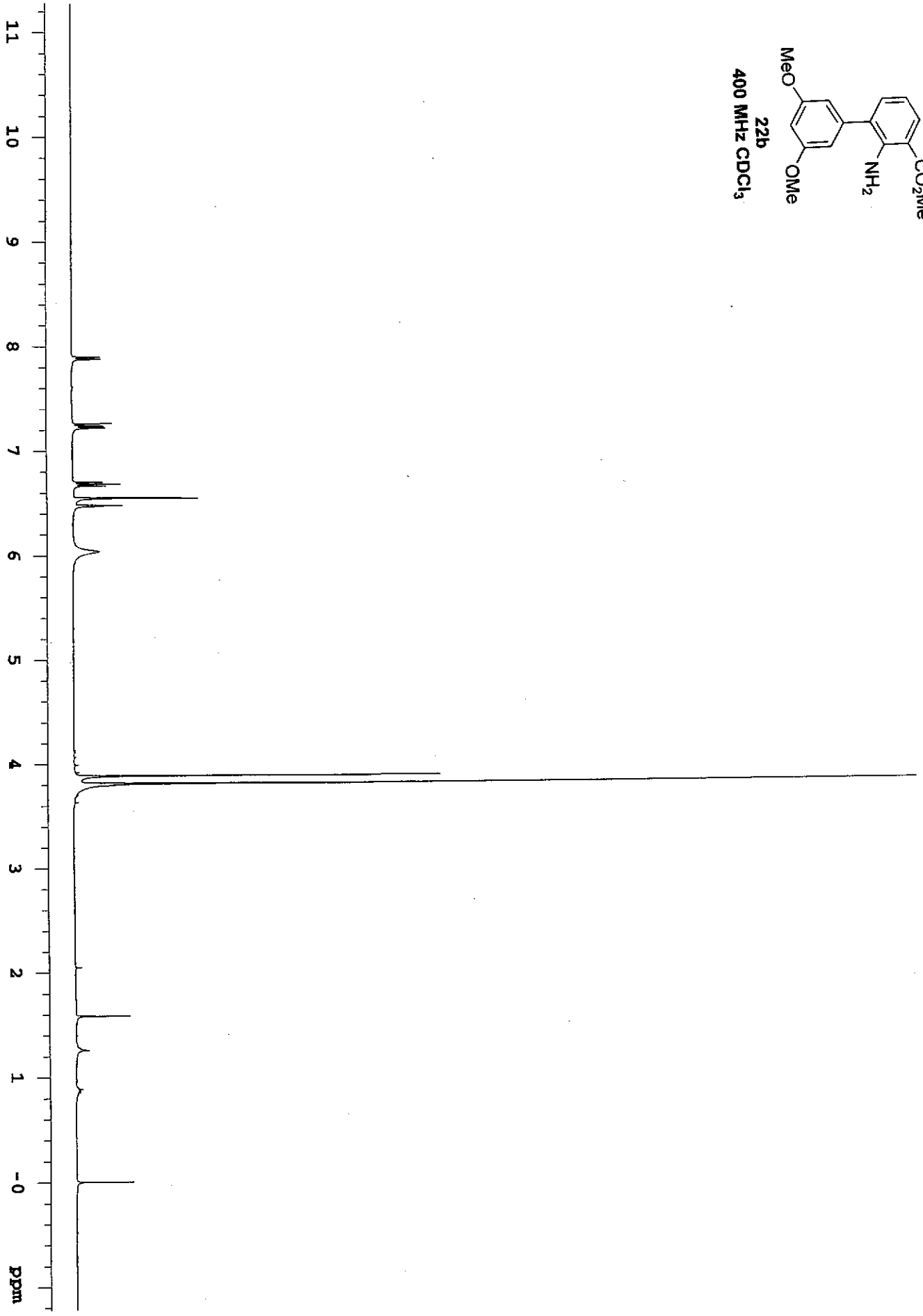
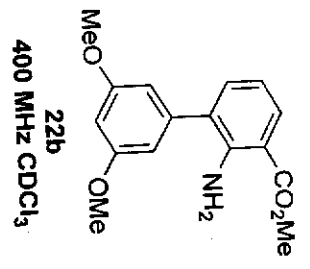


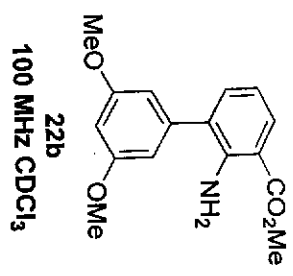
INDEX	FREQUENCY	PPM	HEIGHT
1	16983.531	168.946	6.3
2	16235.850	161.509	33.0
3	15385.172	153.046	12.2
4	13772.318	137.002	14.7
5	13471.720	134.012	40.2
6	12701.151	126.347	12.6
7	12605.021	125.390	37.9
8	12547.801	124.821	47.3
9	11374.400	113.149	12.5
10	10762.522	107.062	6.2
11	10626.719	105.711	87.0
12	10106.394	100.535	41.1
13	7772.563	77.319	344.5
14	7761.119	77.205	27.9
15	7740.519	77.000	355.2
16	7708.476	76.681	346.7
17	5581.401	55.522	84.9
18	5566.142	55.370	7.3
19	-1.790	-0.018	22.2
20	-1912.191	-19.022	-7.6
21	-1944.997	-19.348	-6.2



21b
CDCl₃ 100MHz

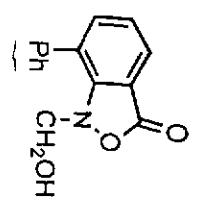






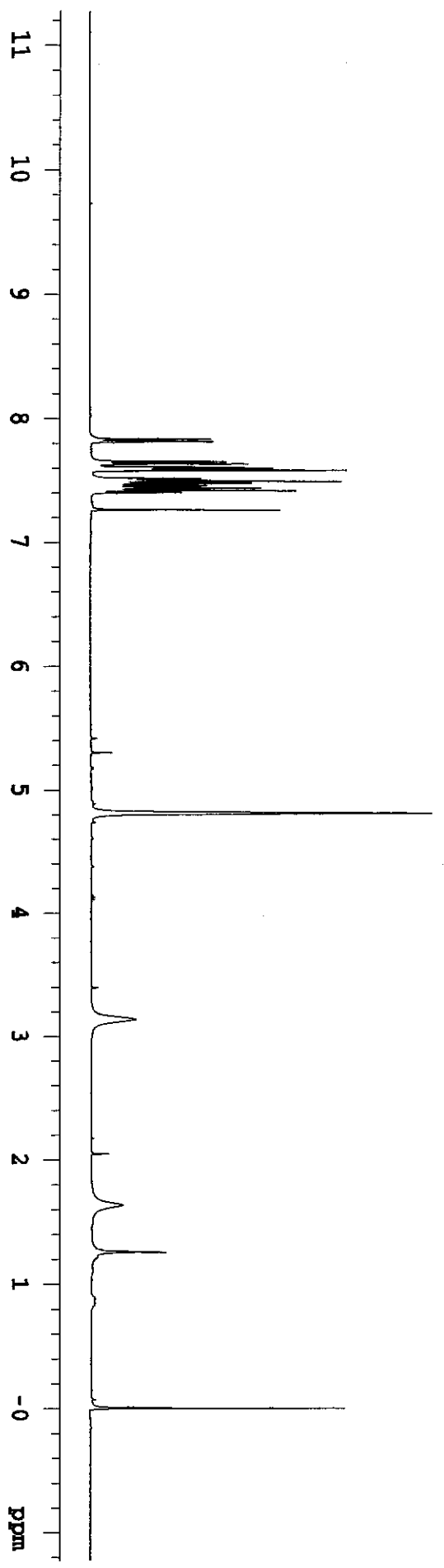
Quon-4-29-5

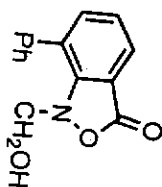
S13



13

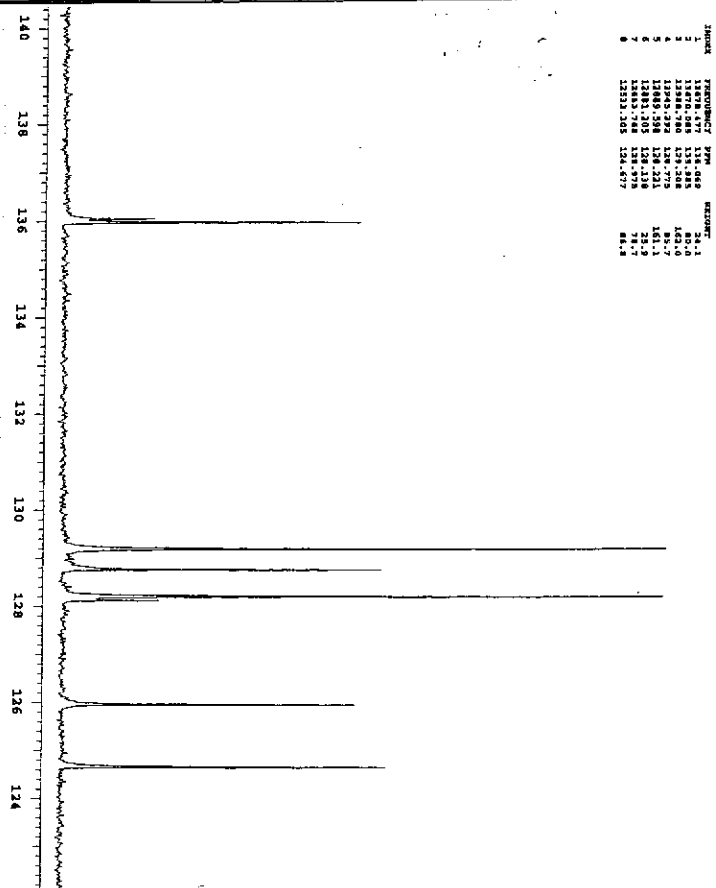
CDCl₃ 400 MHz





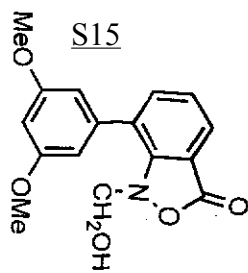
CDCl₃ 100 MHz

INDEX	FREQUENCY	PPM	HEIGHT
1	16948.716	168.600	10.8 ✓
2	15291.561	152.115	9.4 ✓
3	13678.658	136.071	14.8 ✓
4	13670.266	135.987	49.2 (c)
5	12988.940	129.209	99.6 (c)
6	12945.451	128.777	52.7
7	12889.755	128.223	99.1 (c)
8	12881.362	128.139	15.9
9	12663.918	125.976	48.4
10	12533.451	124.678	53.4
11	11688.851	116.277	16.5 ✓
12	7772.864	77.319	163.8
13	7760.356	77.197	8.6
14	7740.519	77.000	171.1
15	7708.475	76.581	169.8
16	7451.356	74.124	51.7
17	2.190	-0.028	6.0



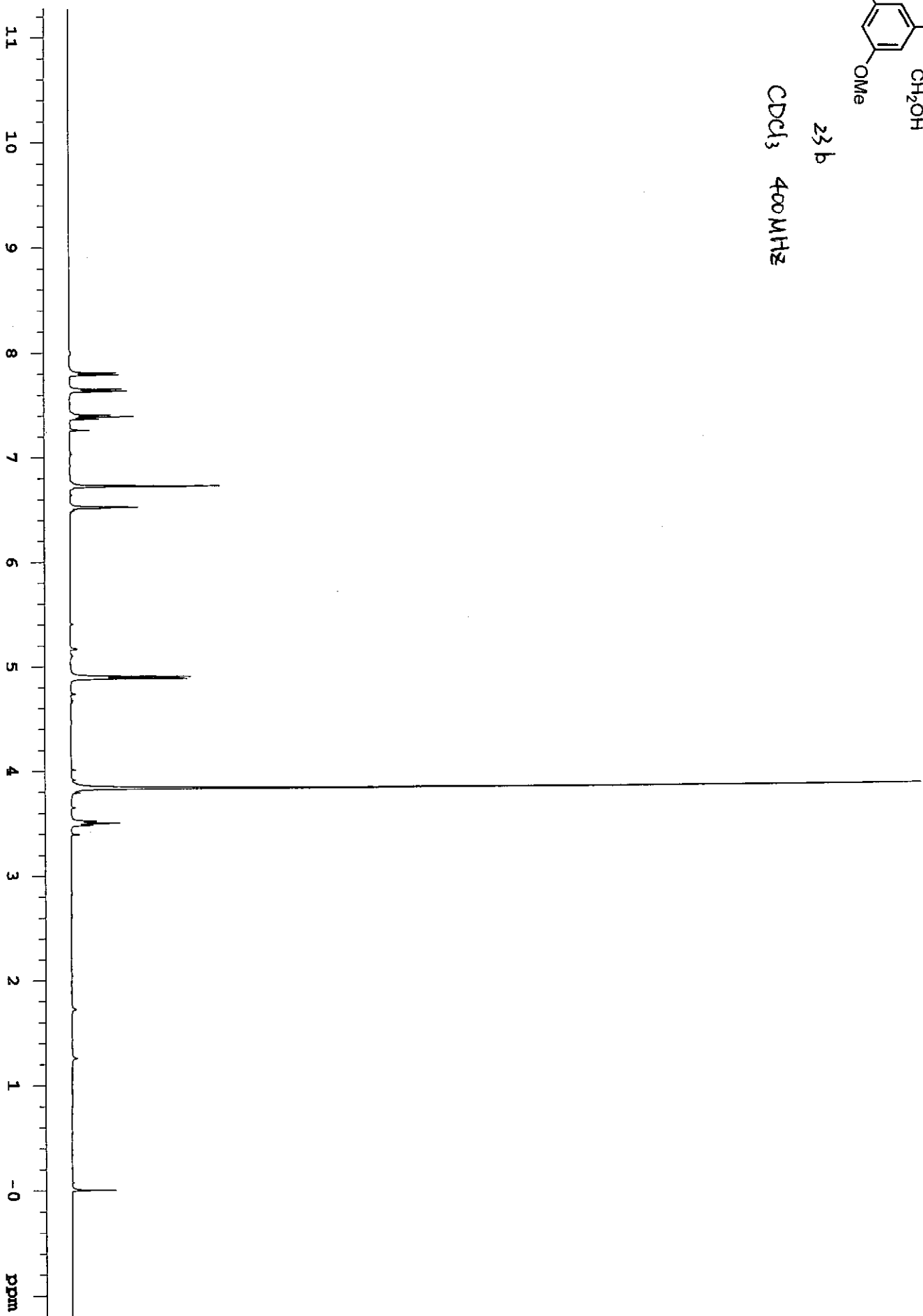
INDEX	FREQUENCY	PPM	HEIGHT
1	1378.617	138.668	24.1
2	1378.617	138.668	162.0
3	1368.780	137.208	181.7
4	1368.780	137.208	21.9
5	1360.772	136.772	78.7
6	1360.772	136.772	78.7
7	1358.768	136.578	88.8
8	1358.768	136.578	88.8

Quan - 4-21-2

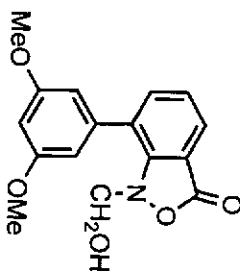


23b

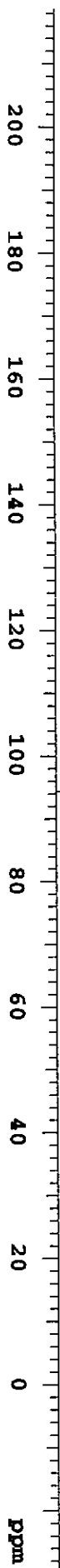
CDCl₃ 400 MHz



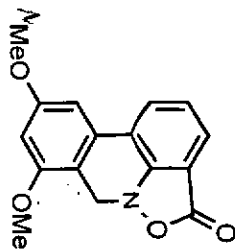
INDEX	FREQUENCY	PPM	HEIGHT
1	16959.726	168.709	24.5
2	16208.971	161.241	87.9 - 2H
3	15385.786	152.058	29.6
4	13863.623	137.911	30.7
5	13645.416	135.740	83.3
6	12870.246	128.029	26.9
7	12645.935	125.797	80.3
8	12542.935	124.773	80.5
9	11681.550	116.204	26.4
10	10679.780	106.239	143.7 - 2H
11	10116.713	100.638	78.5
12	7772.129	77.314	125.6
13	7740.084	76.996	128.9
14	7708.040	76.677	124.8
15	7470.759	74.317	61.7
16	5578.611	55.494	162.0 - 2H



23b
CDCl₃, 100 MHz

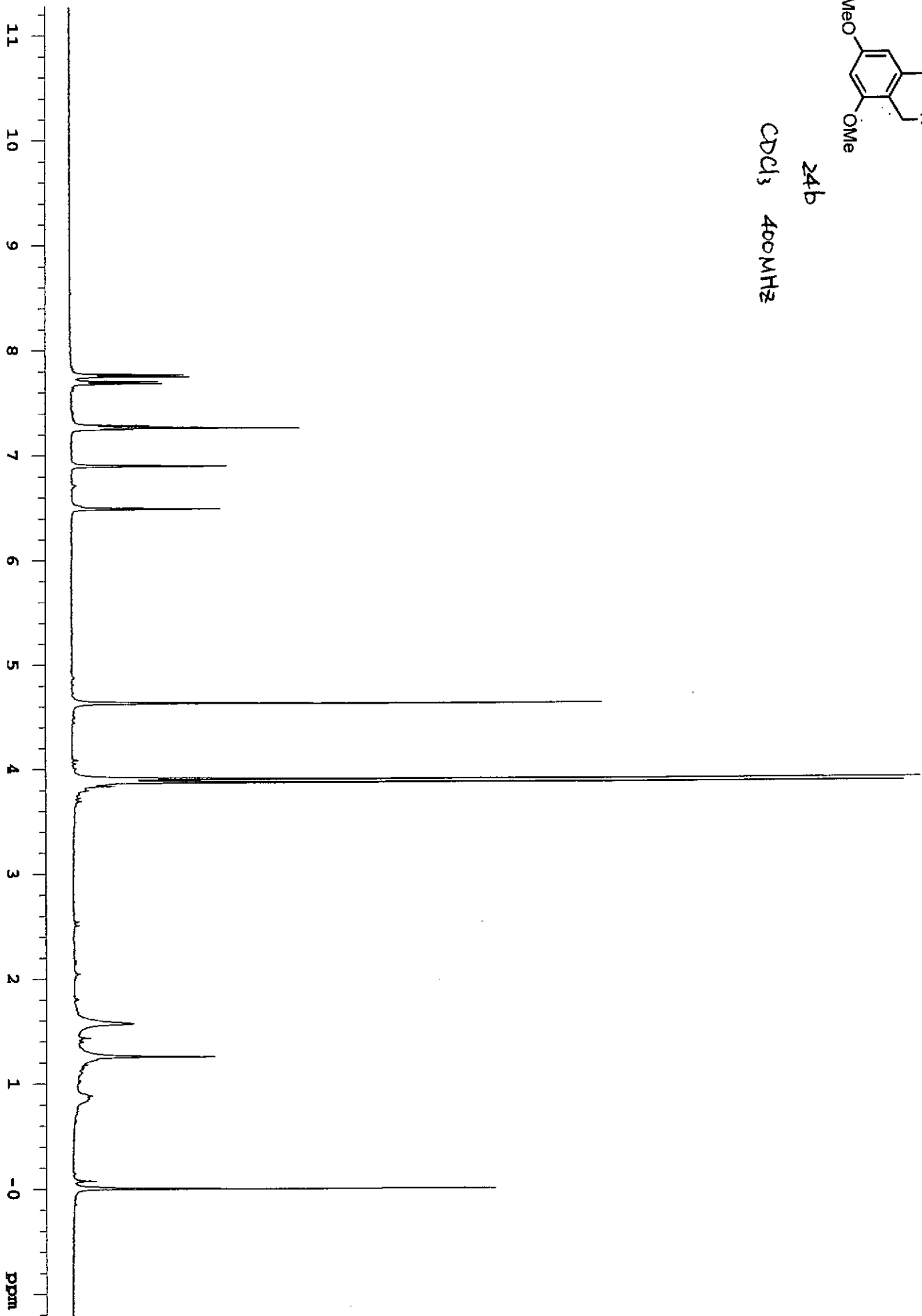


Quan - 4-22-3

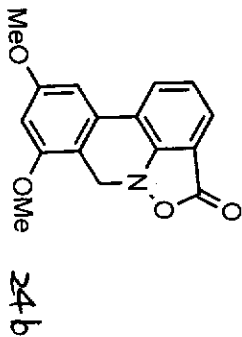


24b

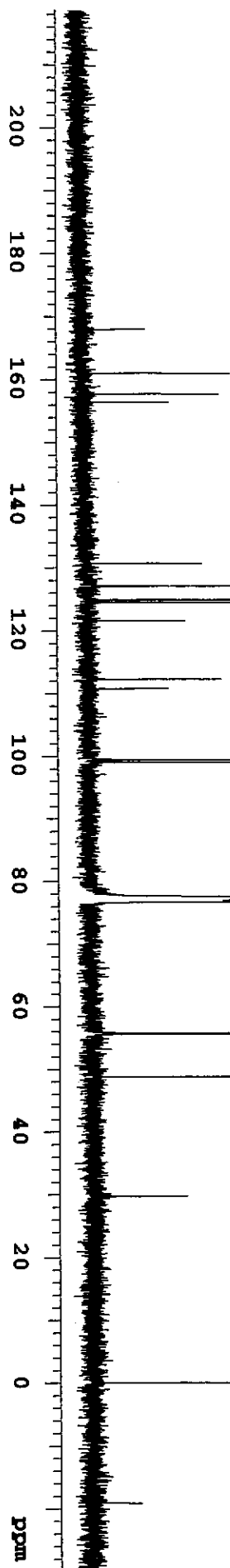
CDCl₃ 400MHz



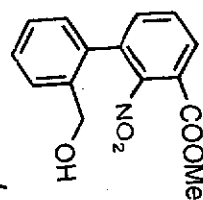
INDEX	FREQUENCY	PPM	HEIGHT
1	16892.585	168.042	9.8
2	16190.660	161.059	23.7
3	15858.771	157.758	21.8
4	15729.067	156.467	13.8
5	13138.046	130.693	19.0
6	12774.112	127.072	68.3
7	12555.905	124.902	70.1
8	12513.942	124.484	70.3
9	12221.727	121.578	16.2
10	11283.283	112.242	22.0
11	11133.743	110.755	13.5
12	9986.247	99.340	63.9
13	9948.098	98.960	74.8
14	7772.129	77.314	386.7
15	7759.921	77.193	40.5
16	7740.084	76.996	400.3
17	7708.040	76.677	395.1
18	5597.685	55.684	73.4
19	5584.715	55.555	70.2
20	4897.285	48.716	75.3
21	2984.538	29.689	16.0
22	-2.462	-0.024	25.4
23	-1924.365	-19.143	8.3



CDCl₃ 100 MHz

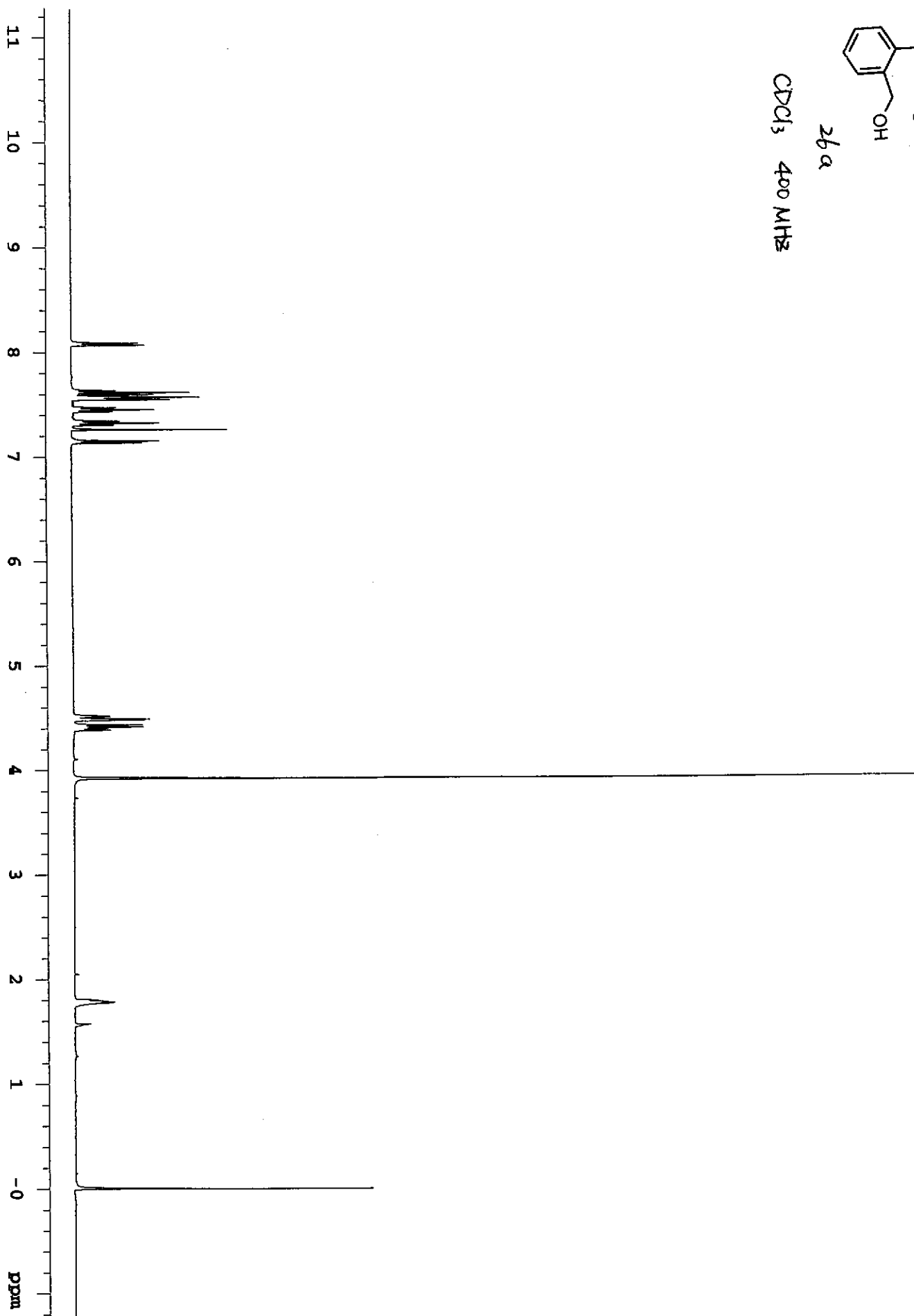


QVAM-4-65-3



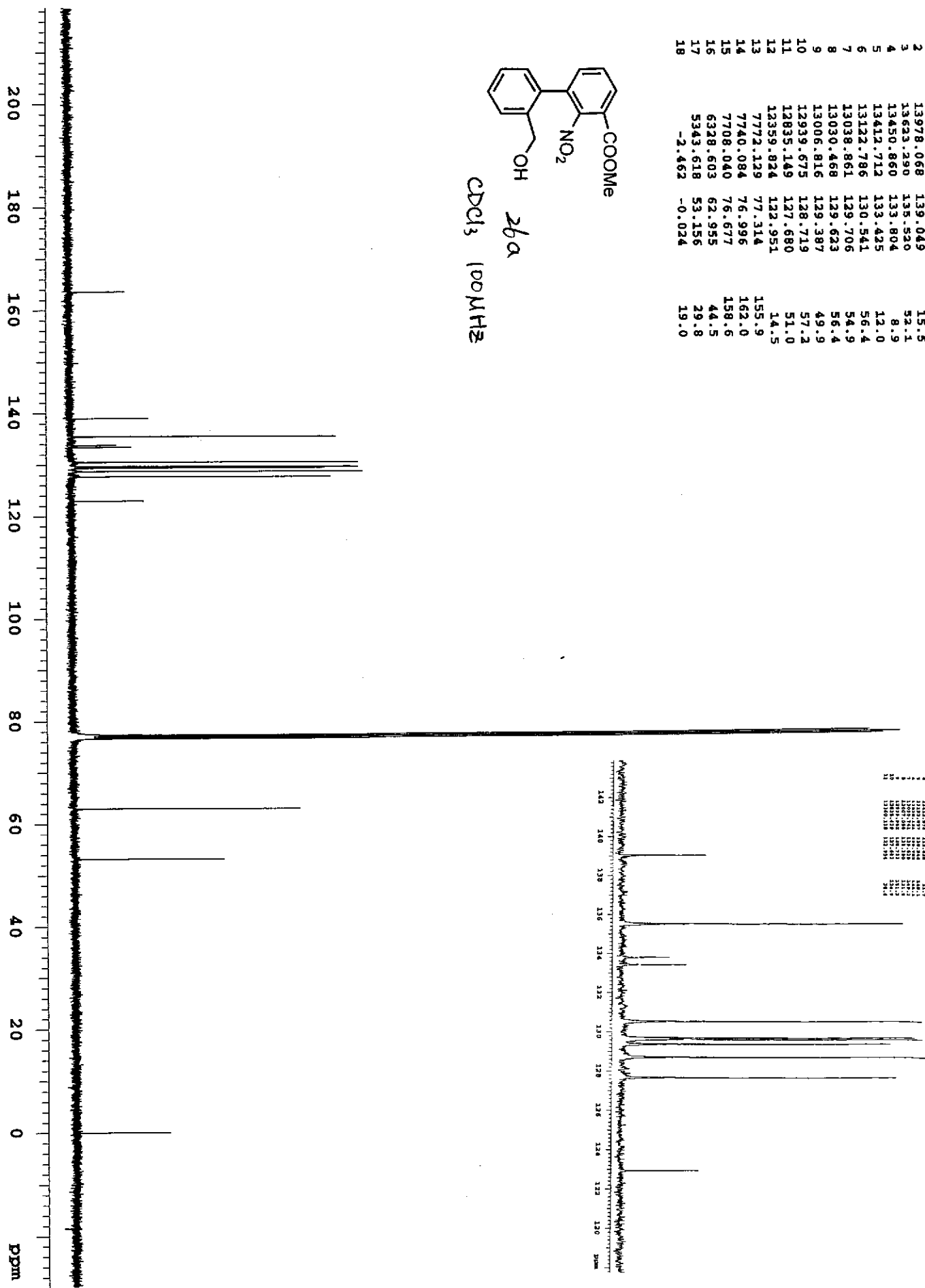
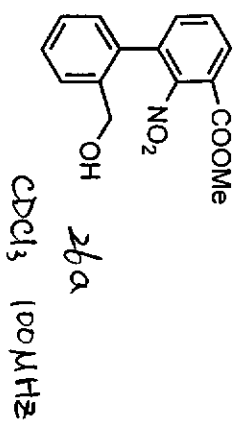
26a

CDCl₃ 400 MHz



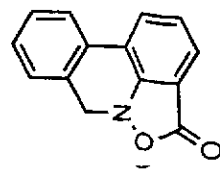
Qvan-4-65-3-carben-1

INDEX	FREQUENCY	PPM	HEIGHT
1	16448.541	163.624	10.8
2	13978.068	139.049	15.5
3	13623.290	135.520	52.1
4	13450.860	133.804	8.9
5	13412.712	133.425	12.0
6	13122.786	130.541	56.4
7	13038.861	129.706	54.9
8	13030.468	129.623	56.4
9	13006.816	129.387	49.9
10	12939.675	128.719	57.2
11	12835.149	127.680	51.0
12	12359.824	122.951	14.5
13	7772.129	77.314	155.9
14	7740.084	76.996	162.0
15	7708.040	76.677	158.6
16	6328.603	62.955	44.5
17	5343.618	53.156	29.8
18	-2.462	-0.024	19.0



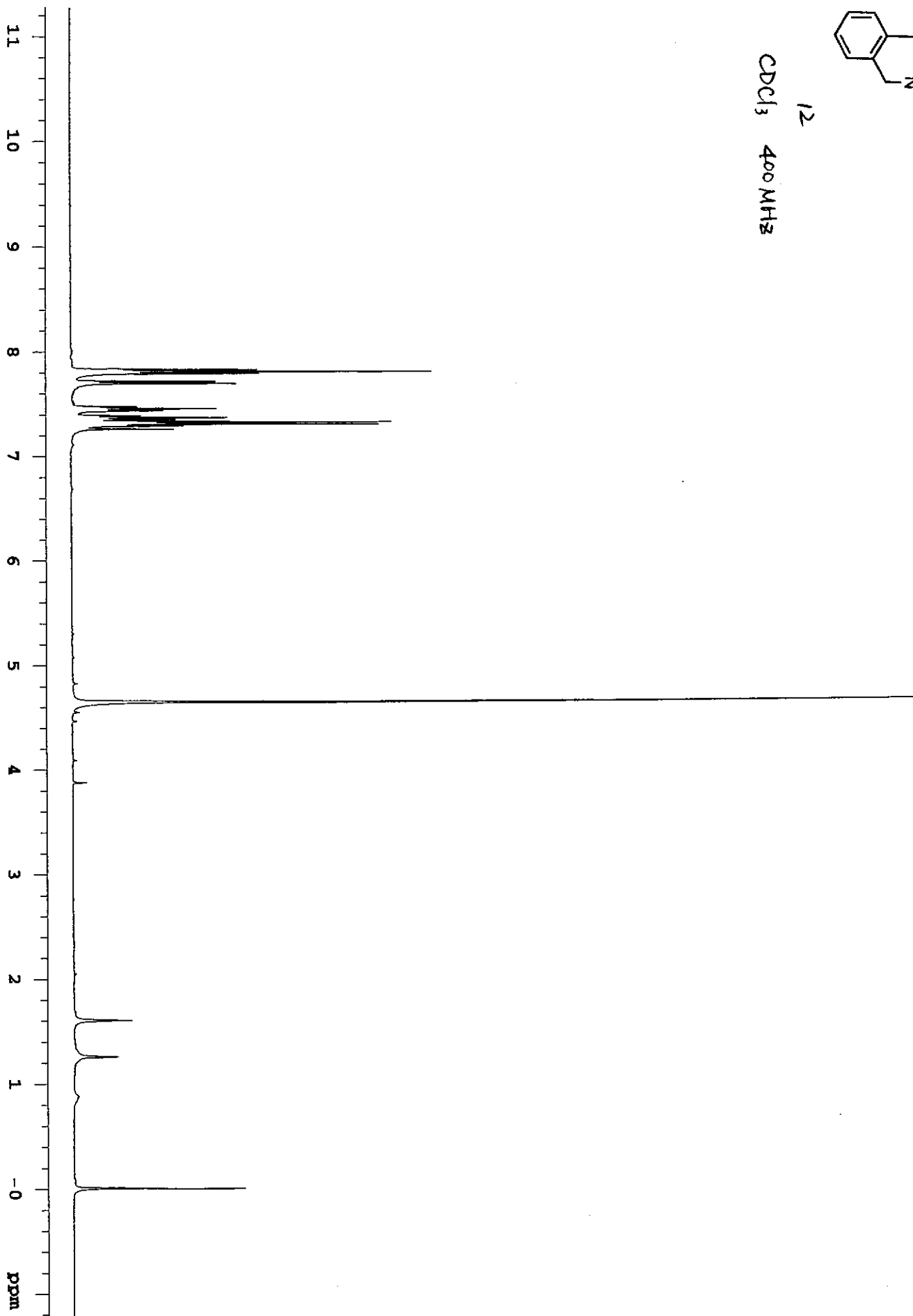
INDEX	FREQUENCY	PPM	HEIGHT
1	16448.541	163.624	10.8
2	13978.068	139.049	15.5
3	13623.290	135.520	52.1
4	13450.860	133.804	8.9
5	13412.712	133.425	12.0
6	13122.786	130.541	56.4
7	13038.861	129.706	54.9
8	13030.468	129.623	56.4
9	13006.816	129.387	49.9
10	12939.675	128.719	57.2
11	12835.149	127.680	51.0
12	12359.824	122.951	14.5
13	7772.129	77.314	155.9
14	7740.084	76.996	162.0
15	7708.040	76.677	158.6
16	6328.603	62.955	44.5
17	5343.618	53.156	29.8
18	-2.462	-0.024	19.0

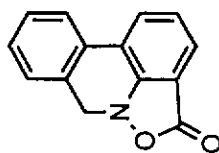
Quan - 4-72-1



12

CDCl₃ 400 MHz

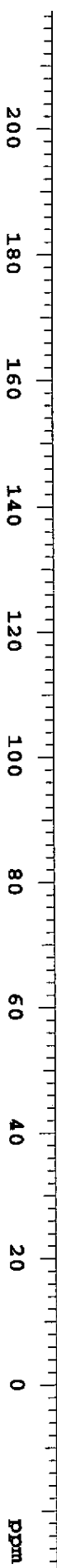


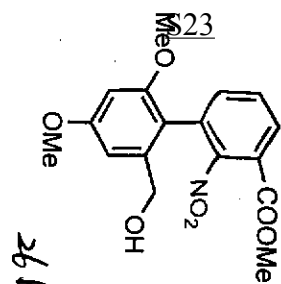


12

CDCl₃ 100MHz

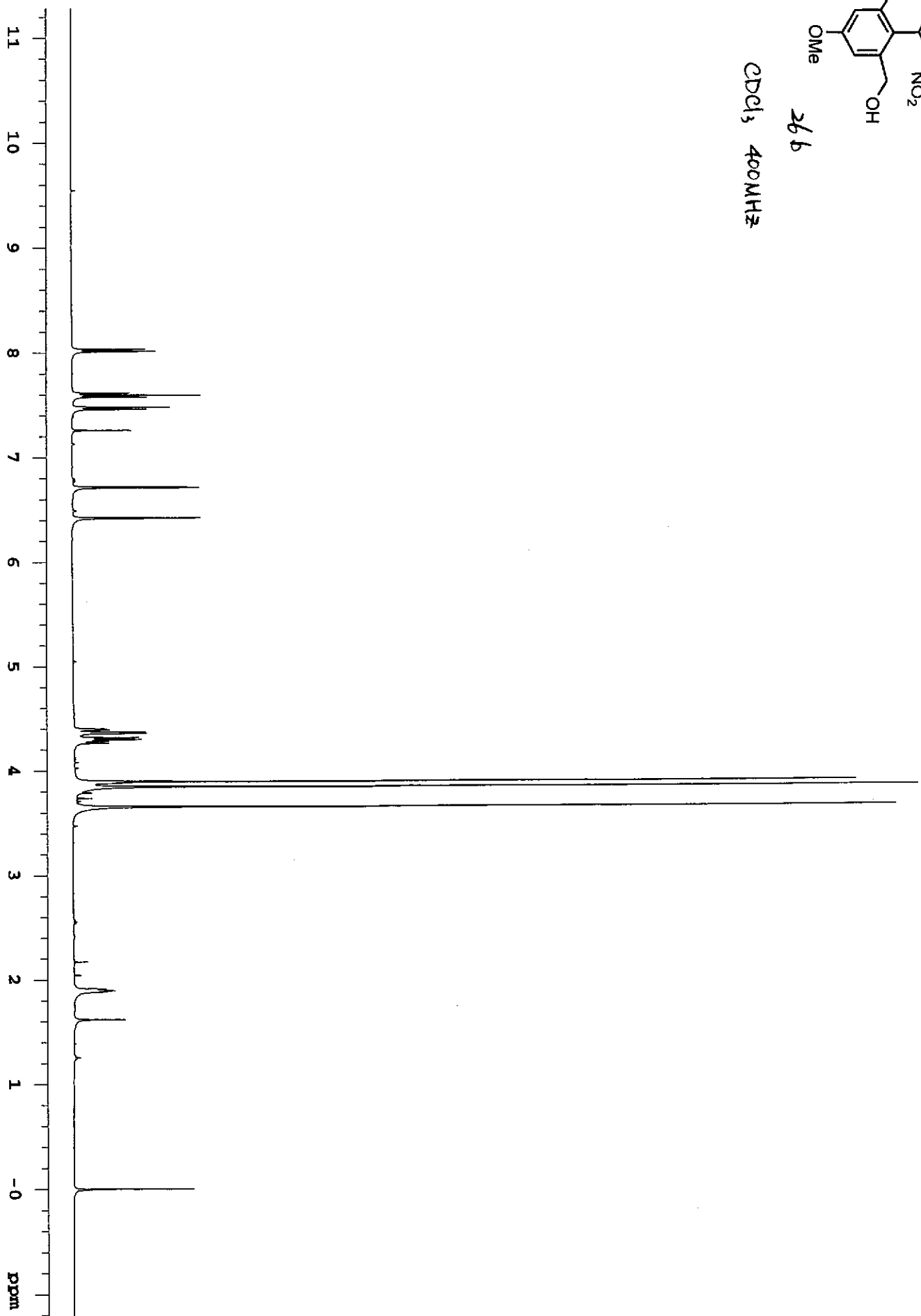
INDEX	FREQUENCY	PPM	HEIGHT
1	16877.761	167.894	11.8
2	15727.976	156.456	11.6
3	13184.258	131.152	19.1
4	13002.673	129.346	54.7
5	12997.333	129.293	63.5
6	12987.414	129.194	17.7
7	12908.829	128.413	56.0
8	12766.918	127.001	60.1
9	12605.170	125.392	48.8
10	12501.407	124.360	64.2
11	12380.096	123.153	57.1
12	12230.555	121.665	13.6
13	11170.800	111.123	13.0
14	7772.564	77.319	161.4
15	7761.119	77.205	9.0
16	7740.519	77.000	162.0
17	7709.338	76.689	157.3
18	5559.972	55.309	62.7





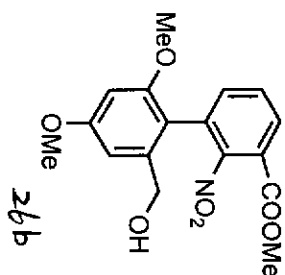
CDCl₃, 400MHz

266

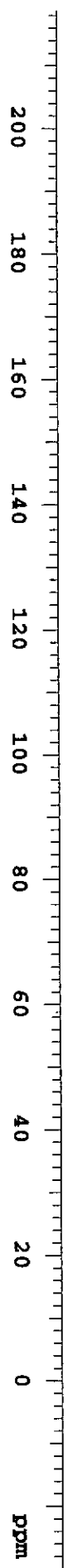


CDCl₃ - 4-111-2 - carbem

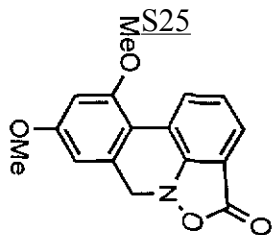
INDEX	FREQUENCY	PPM	HEIGHT
1	16482.874	163.966	27.7
2	16240.252	161.552	32.1
3	15883.949	158.008	44.8
4	15137.771	150.585	5.7
5	14246.631	141.721	37.0
6	13743.838	136.719	109.1
7	13126.601	130.579	38.5
8	13093.794	130.253	108.3
9	13064.038	129.957	106.0
10	12394.157	123.293	31.8
11	11531.246	114.709	20.0
12	10474.543	104.197	96.6
13	9851.965	98.004	113.1
14	7772.129	77.314	151.1
15	7740.084	76.996	162.0
16	7708.040	76.677	161.6
17	6322.500	62.894	83.8
18	5606.841	55.775	96.3
19	5569.455	55.403	84.7
20	5331.411	53.035	80.1
21	-3.987	-0.040	11.2



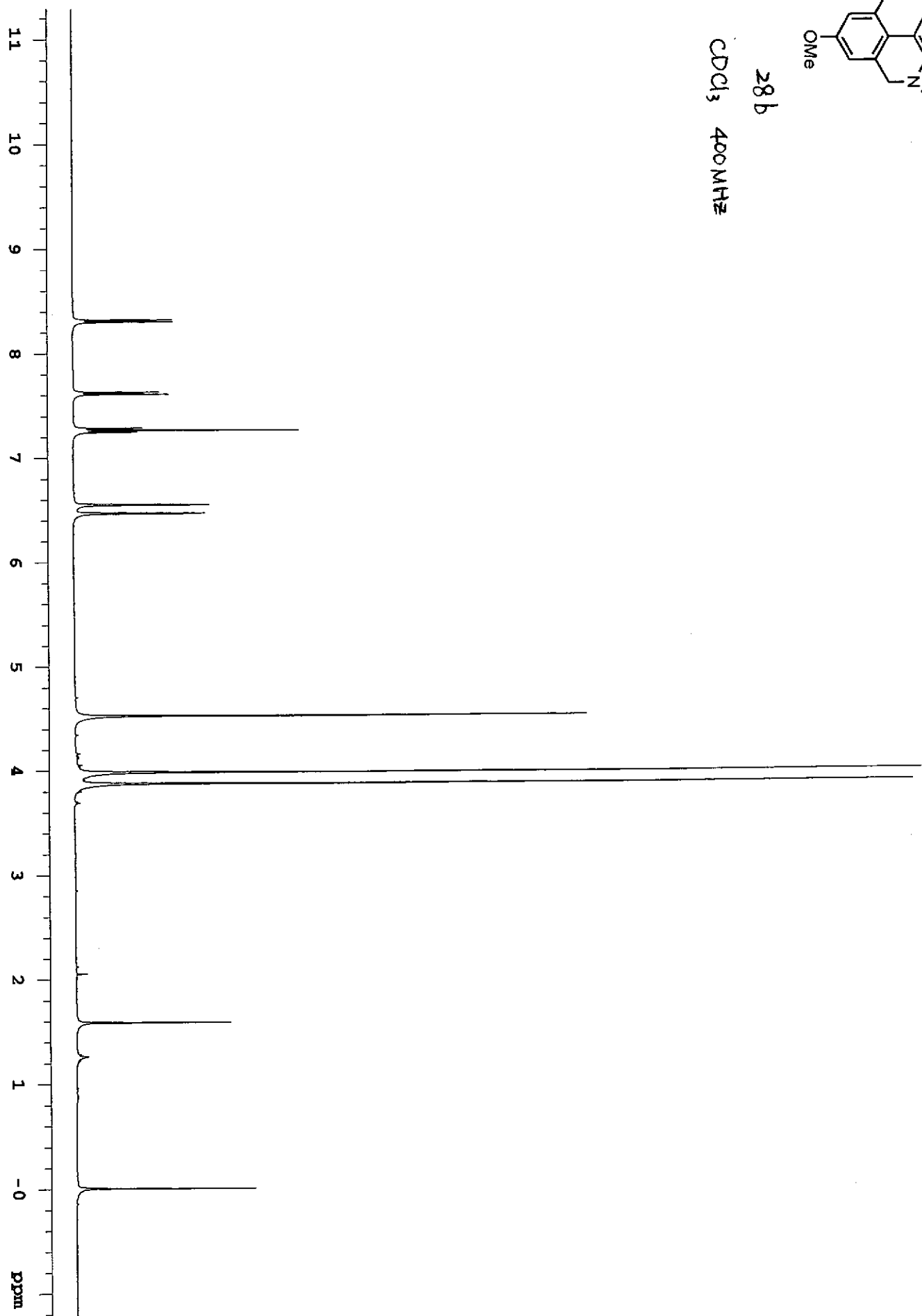
CDCl₃ 100MHz
26b



Quan - 4-113-2

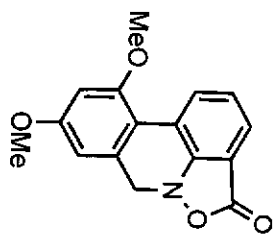


CDCl₃ 400MHz
28b



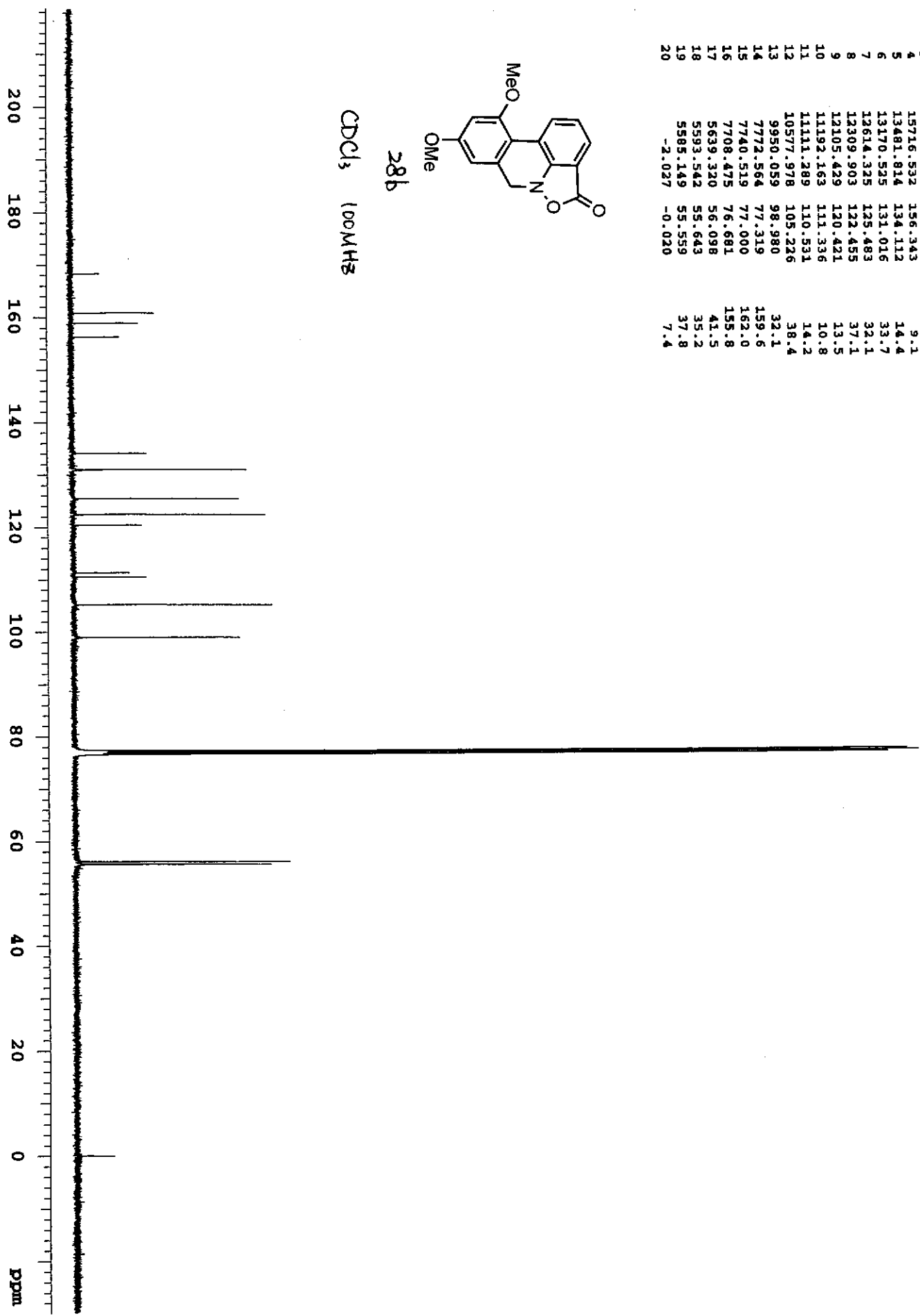
Quan - 4 - 113 - 2 - carbon.

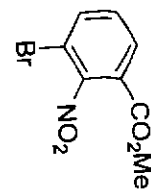
INDEX	FREQUENCY PPM	PPM	HEIGHT
1	16931.168	168.425	5.4
2	16175.072	160.904	16.1
3	15978.991	158.953	12.9
4	15716.532	156.343	9.1
5	13481.814	134.112	14.4
6	13170.525	131.016	33.7
7	12614.325	125.483	32.1
8	12309.903	122.455	37.1
9	12105.429	120.421	13.5
10	11192.163	111.336	10.8
11	11111.289	110.531	14.2
12	10577.978	105.226	38.4
13	9950.059	98.980	32.1
14	7772.564	77.319	159.6
15	7740.519	77.000	162.0
16	7708.475	76.681	155.8
17	5639.320	56.098	41.5
18	5593.542	55.643	35.2
19	5585.149	55.559	37.8
20	-2.027	-0.020	7.4



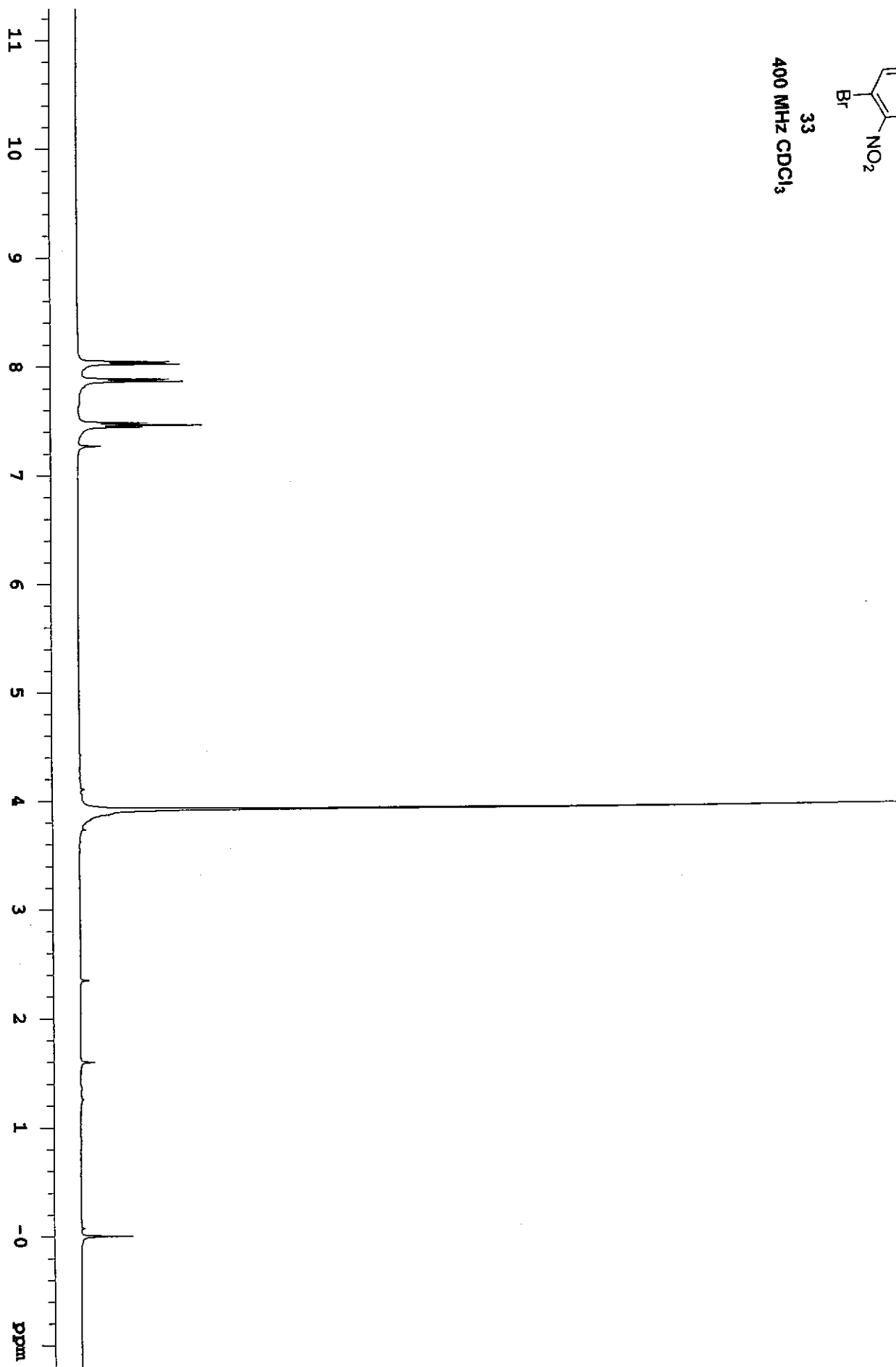
28b

CDCl₃ 100MHz

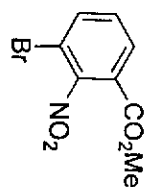




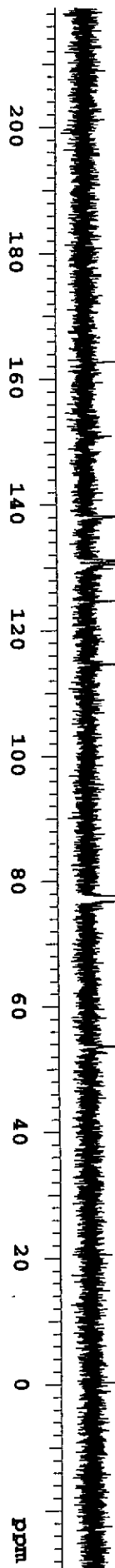
33
400 MHz CDCl₃

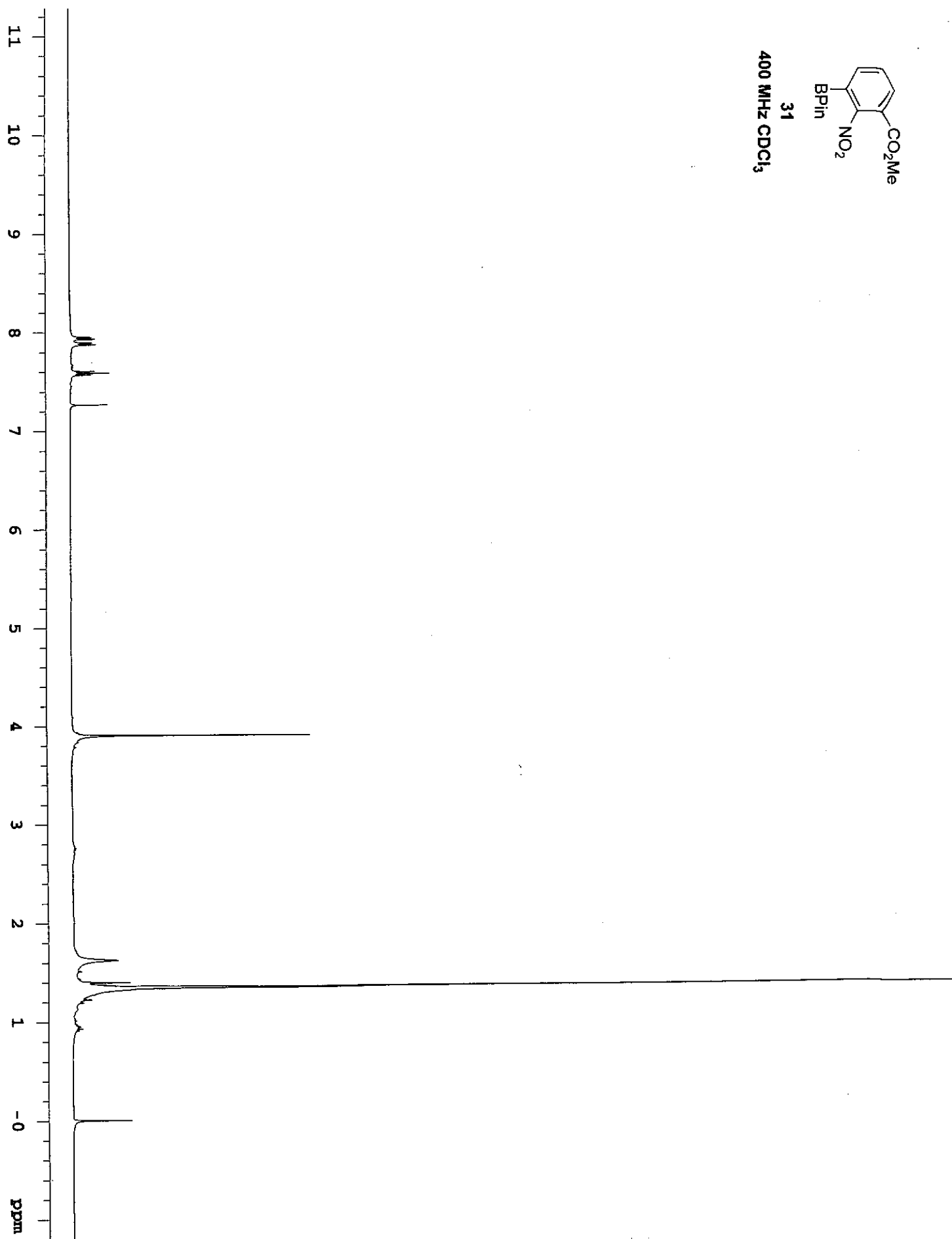
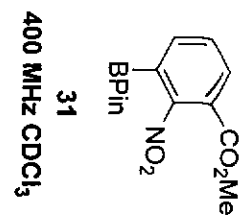


INDEX	FREQUENCY	PPM	HEIGHT
1	16355.270	162.697	22.6
2	13884.797	138.121	162.0
3	13179.819	131.108	156.9
4	13131.834	130.531	156.2
5	12531.301	124.657	28.5
6	11520.375	114.601	44.9
7	7797.117	77.563	133.3
8	7765.072	77.244	137.4
9	7733.791	76.933	136.1
10	5385.392	53.572	104.3

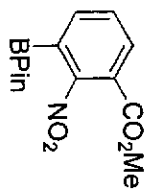


33
100 MHz CDCl₃

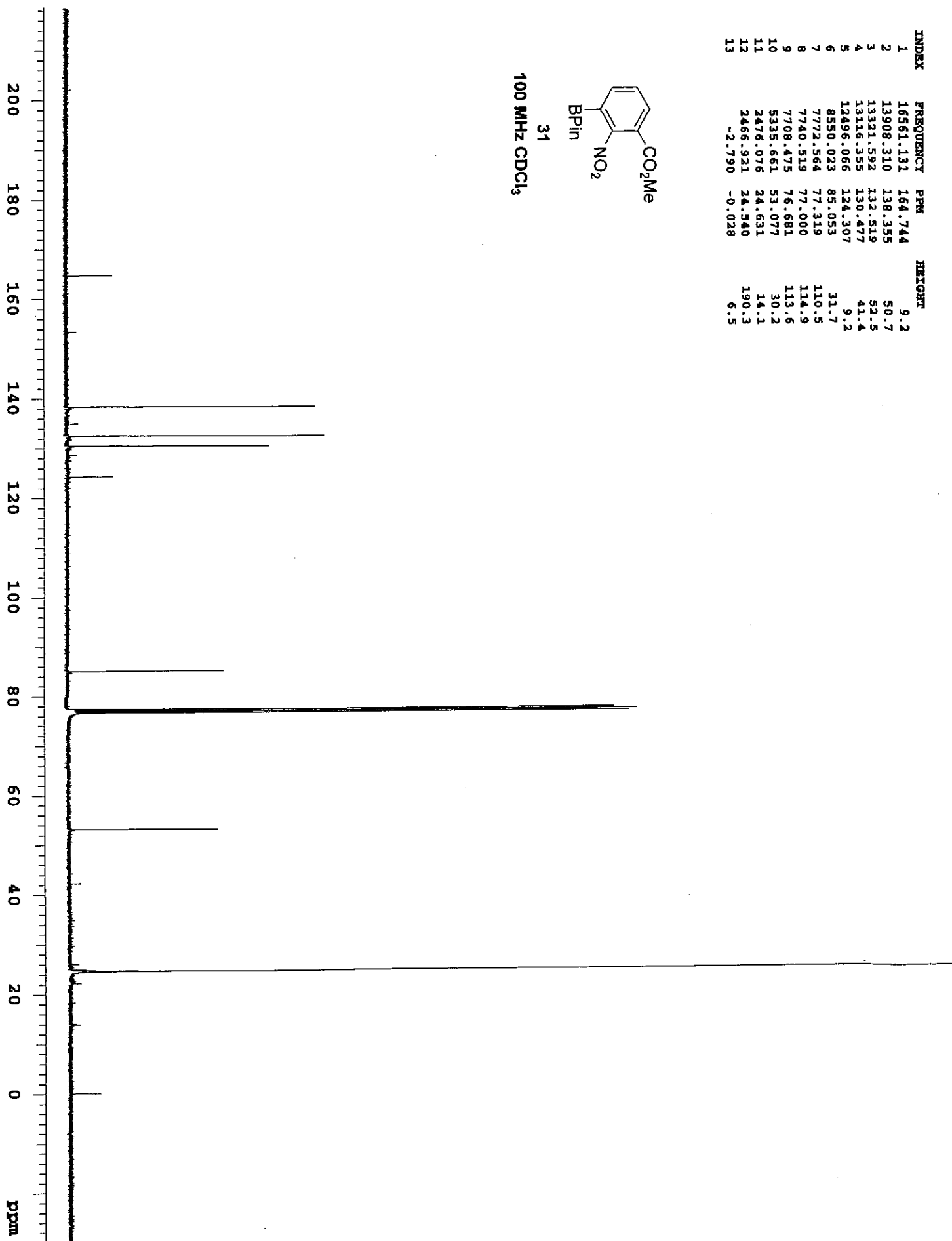


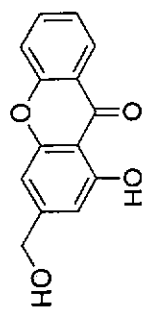


INDEX	FREQUENCY	PPM	HEIGHT
1	16561.131	164.744	9.2
2	13908.310	138.355	50.7
3	13321.592	132.519	52.5
4	13116.355	130.477	41.4
5	12496.066	124.307	9.2
6	8550.023	85.053	31.7
7	7772.564	77.319	110.5
8	7740.519	77.000	114.9
9	7708.475	76.681	113.6
10	5335.661	53.077	30.2
11	2476.076	24.631	14.1
12	2466.921	24.540	190.3
13	-2.790	-0.028	6.5

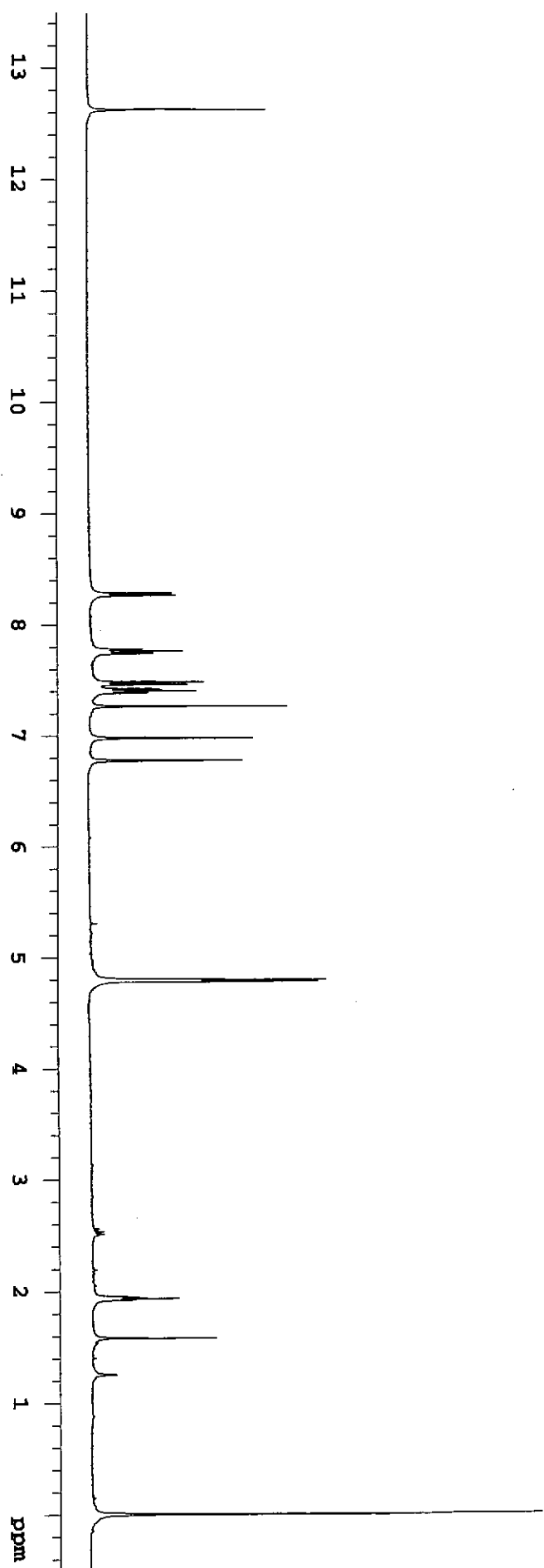


100 MHz CDCl₃

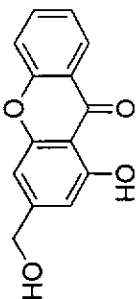




37b
400 MHz CDCl₃

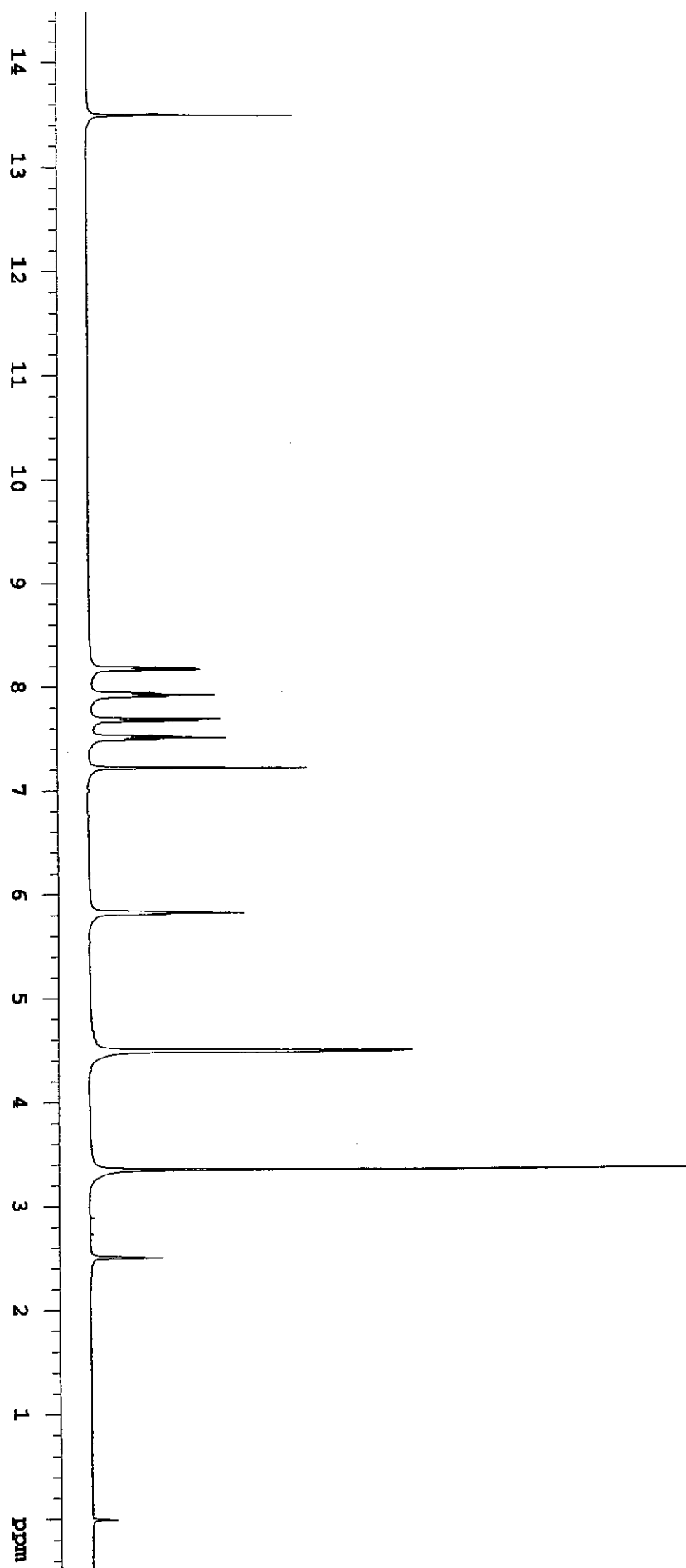
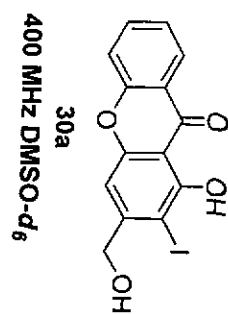


INDEX	FREQUENCY	PPM	HEIGHT
1	18292.622	181.969	6.3
2	16277.637	161.924	11.5
3	15728.304	156.460	8.5
4	15700.838	156.186	7.3
5	15207.201	151.276	11.6
6	13624.816	135.535	31.7
7	12660.431	125.942	25.7
8	12475.794	124.105	29.4
9	12121.779	120.583	8.2
10	11849.402	117.874	31.1
11	10858.313	108.015	6.4
12	10836.950	107.802	29.5
13	10491.328	104.364	26.6
14	7772.129	77.314	151.9
15	7740.084	76.996	160.6
16	7709.040	76.677	162.0
17	6486.537	64.526	24.1
18	-2.461	-0.024	8.3

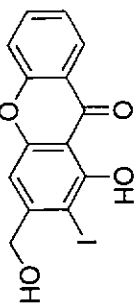


37b
100 MHz CDCl₃



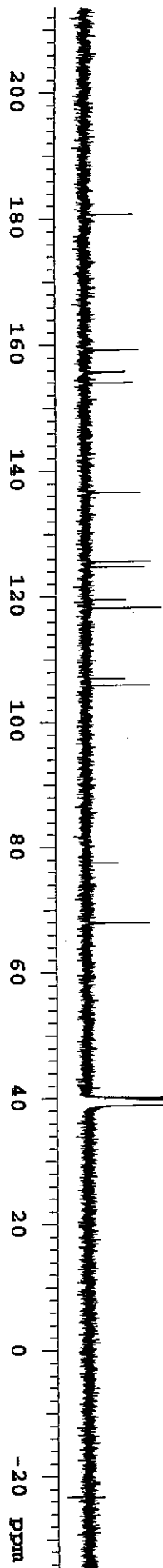


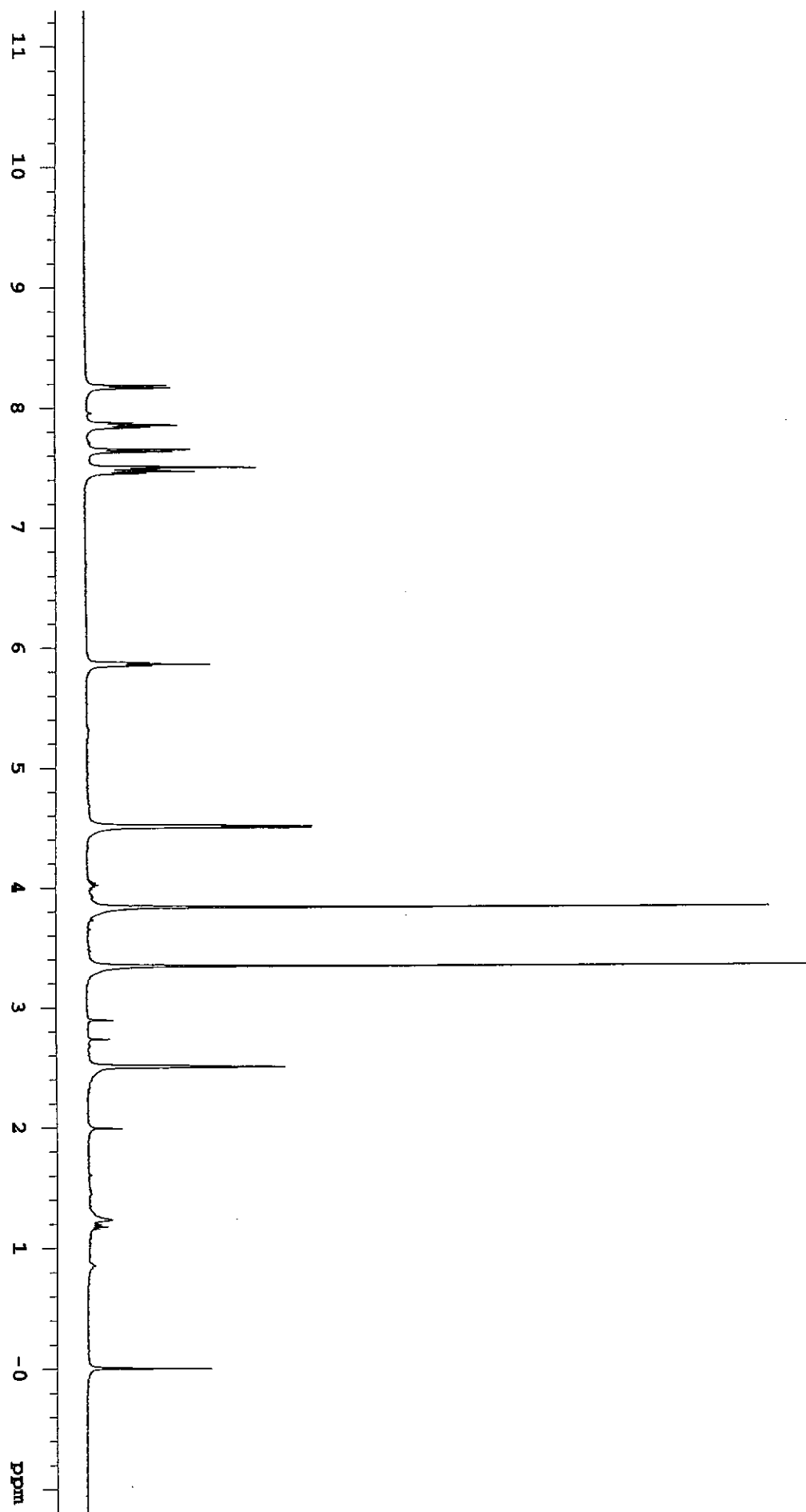
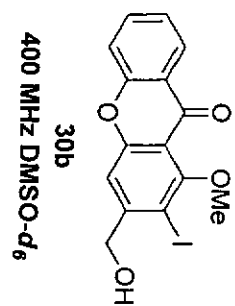
INDEX	FREQUENCY	PPM	HEIGHT
1	18179.170	180.839	7.8
2	16010.830	159.269	8.6
3	15668.259	155.862	6.4
4	15642.319	155.604	6.3
5	15488.200	154.070	7.7
6	13731.097	136.591	8.8
7	12623.275	125.571	10.5
8	12542.164	124.774	9.5
9	12017.483	119.545	6.5
10	11883.201	118.209	12.3
11	10753.253	106.969	6.3
12	10641.861	105.861	10.3
13	7790.669	77.498	5.2
14	6823.232	67.875	10.1
15	4033.841	40.127	20.8
16	4013.241	39.922	66.6
17	3991.878	39.710	136.1
18	3971.278	39.505	162.0
19	3949.915	39.292	139.4
20	3929.315	39.087	72.1
21	3907.952	38.875	25.5



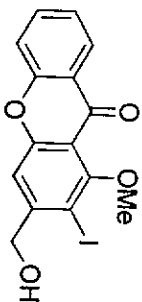
30a

100 MHz DMSO-d₆



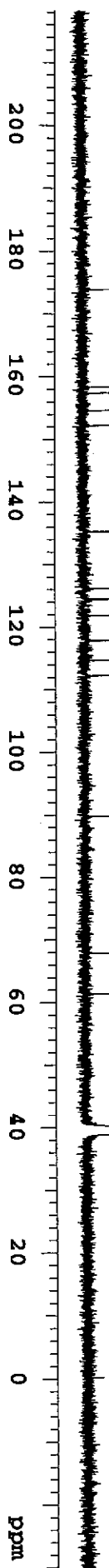


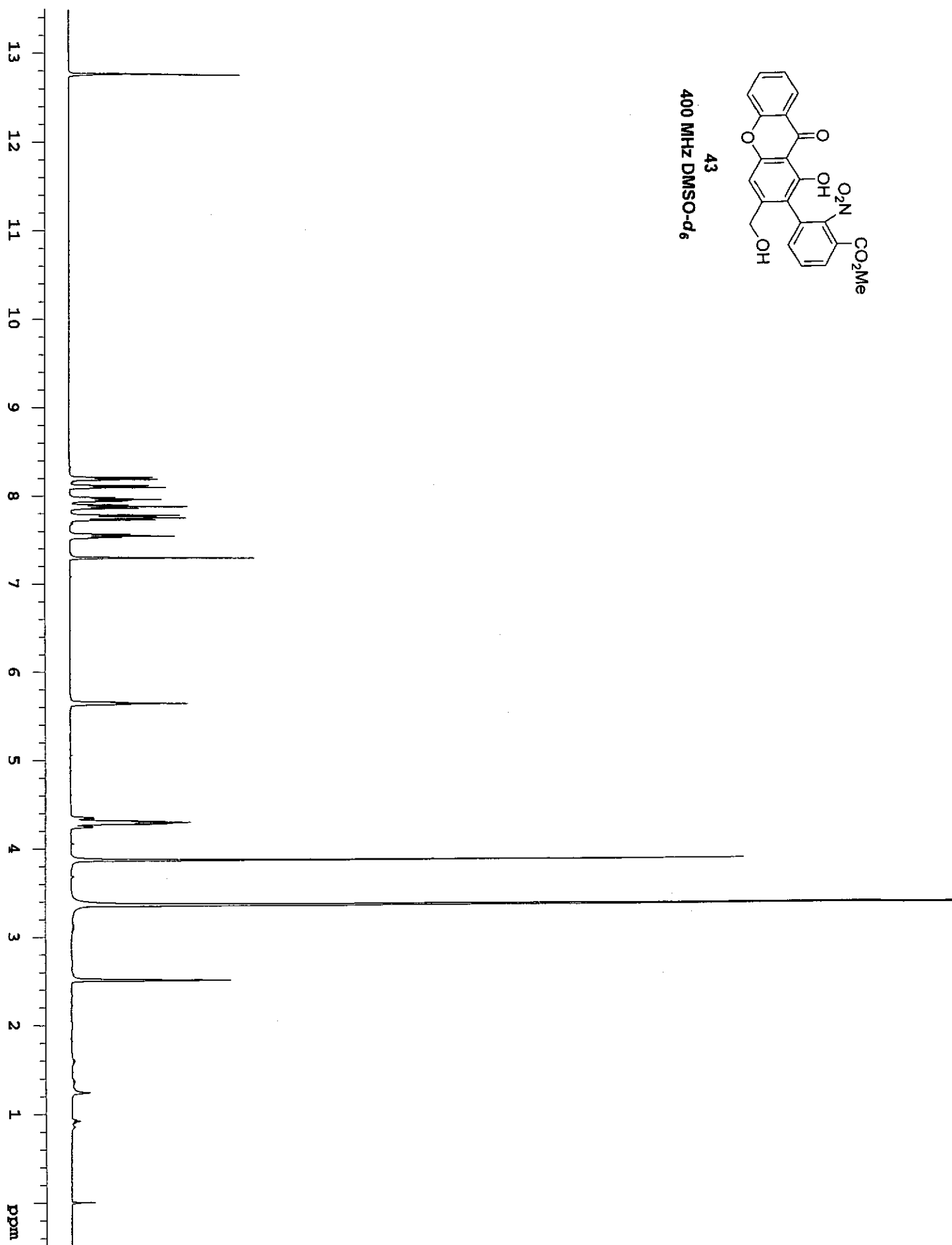
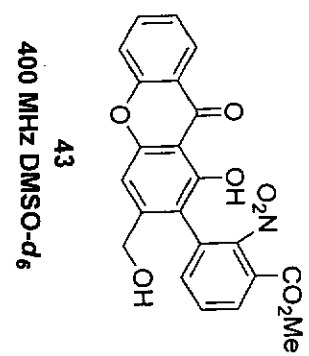
INDEX	FREQUENCY	PPM	HEIGHT
1	17480.281	173.887	7.9
2	15916.208	158.328	7.9
3	15832.363	157.395	9.6
4	15540.067	154.586	9.2
5	15302.023	152.218	12.8
6	13596.801	135.256	17.5
7	12683.534	126.171	16.3
8	12509.579	124.440	15.0
9	12250.172	121.860	11.0
10	11843.512	117.815	18.9
11	11525.357	114.650	7.3
12	11280.446	112.213	17.9
13	9019.787	89.725	8.6
14	6820.166	67.844	15.5
15	6160.966	61.287	14.6
16	4033.826	40.127	88.1
17	4013.226	39.922	271.3
18	3991.863	39.709	539.5
19	3971.263	39.505	637.5
20	3949.900	39.292	542.2
21	3929.300	39.087	271.3
22	3907.937	38.875	89.1



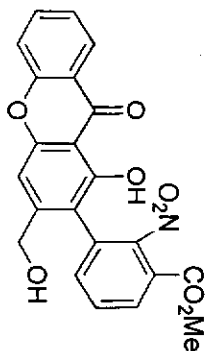
30b

100 MHz DMSO-d₆

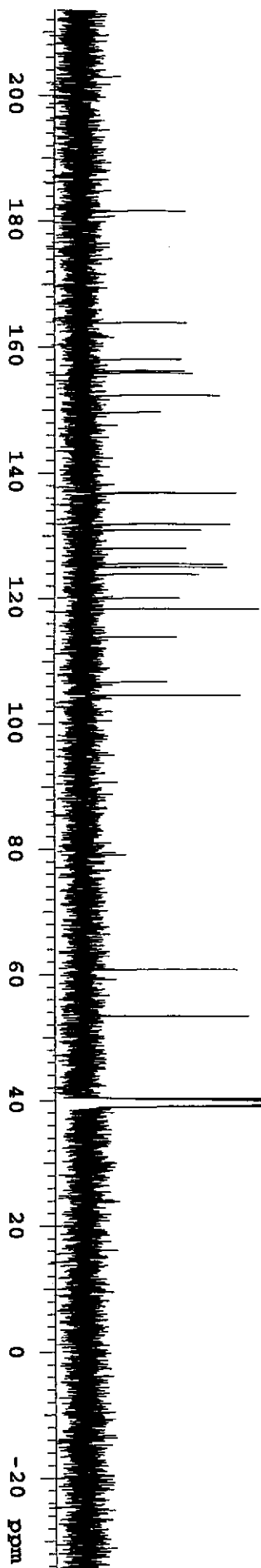


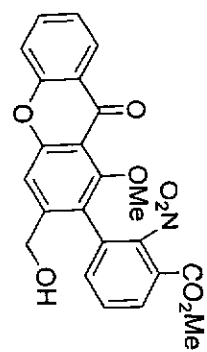


INDEX	FREQUENCY	PPM	HEIGHT
1	18246.310	181.507	16.3
2	16464.029	163.778	16.5
3	15876.548	157.934	15.7
4	15694.200	156.120	16.1
5	15659.867	155.778	17.5
6	15305.089	152.249	22.0
7	15029.659	149.509	12.1
8	13747.882	136.758	24.5
9	13739.489	136.675	21.6
10	13245.090	131.757	23.6
11	13152.008	130.831	18.9
12	12856.741	127.894	16.3
13	12610.305	125.442	22.3
14	12556.897	124.911	23.0
15	12444.742	123.795	18.4
16	12057.157	119.940	15.3
17	11887.779	118.255	28.2
18	11436.105	113.762	14.8
19	10715.105	106.590	13.3
20	10502.238	104.472	25.1
21	6101.469	60.695	24.5
22	5358.344	53.303	26.4
23	4034.603	40.135	85.1
24	4013.240	39.922	255.0
25	3992.640	39.717	520.4
26	3971.277	39.505	609.4
27	3950.677	39.300	522.0
28	3929.314	39.087	262.4
29	3908.715	38.882	87.0

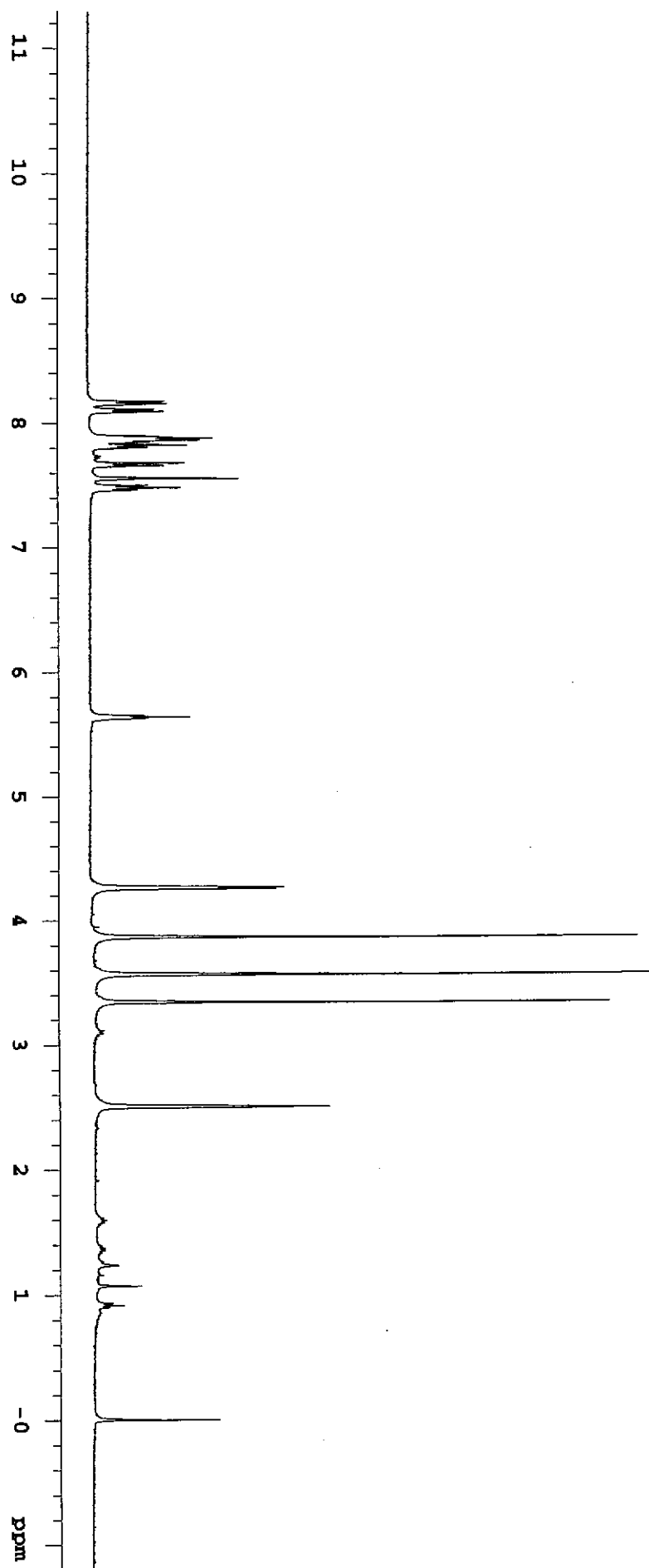


100 MHz DMSO-d₆

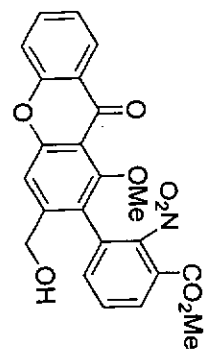




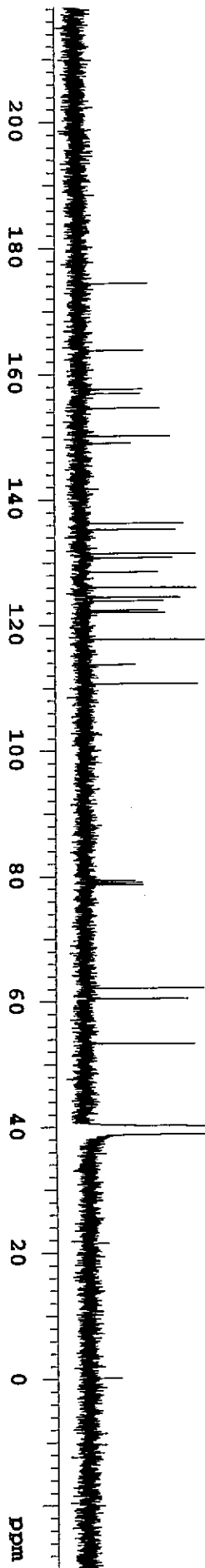
46

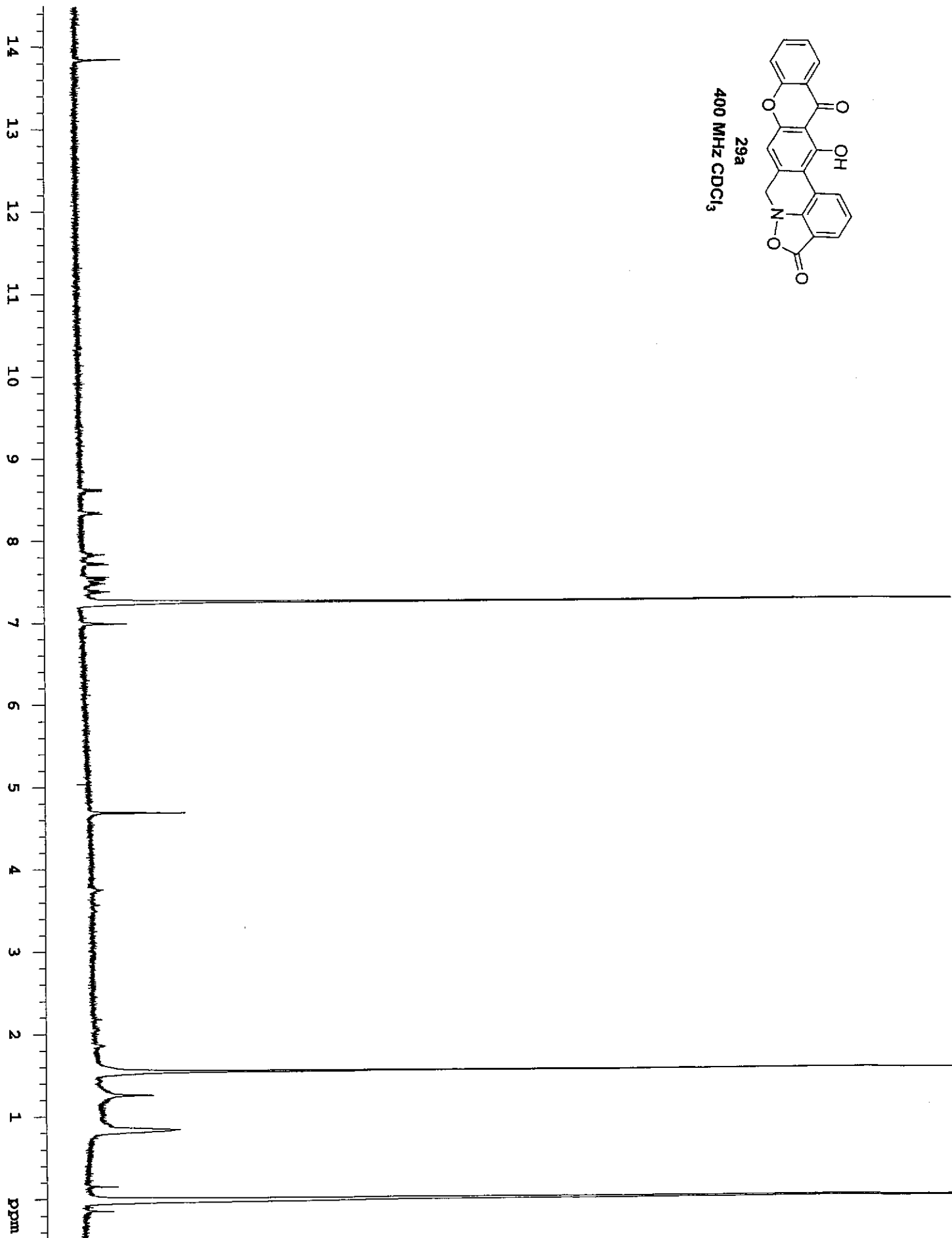
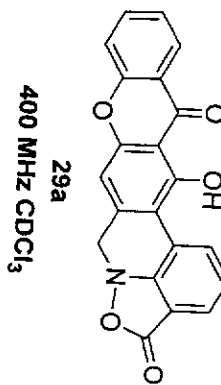
400 MHz DMSO-*d*₆

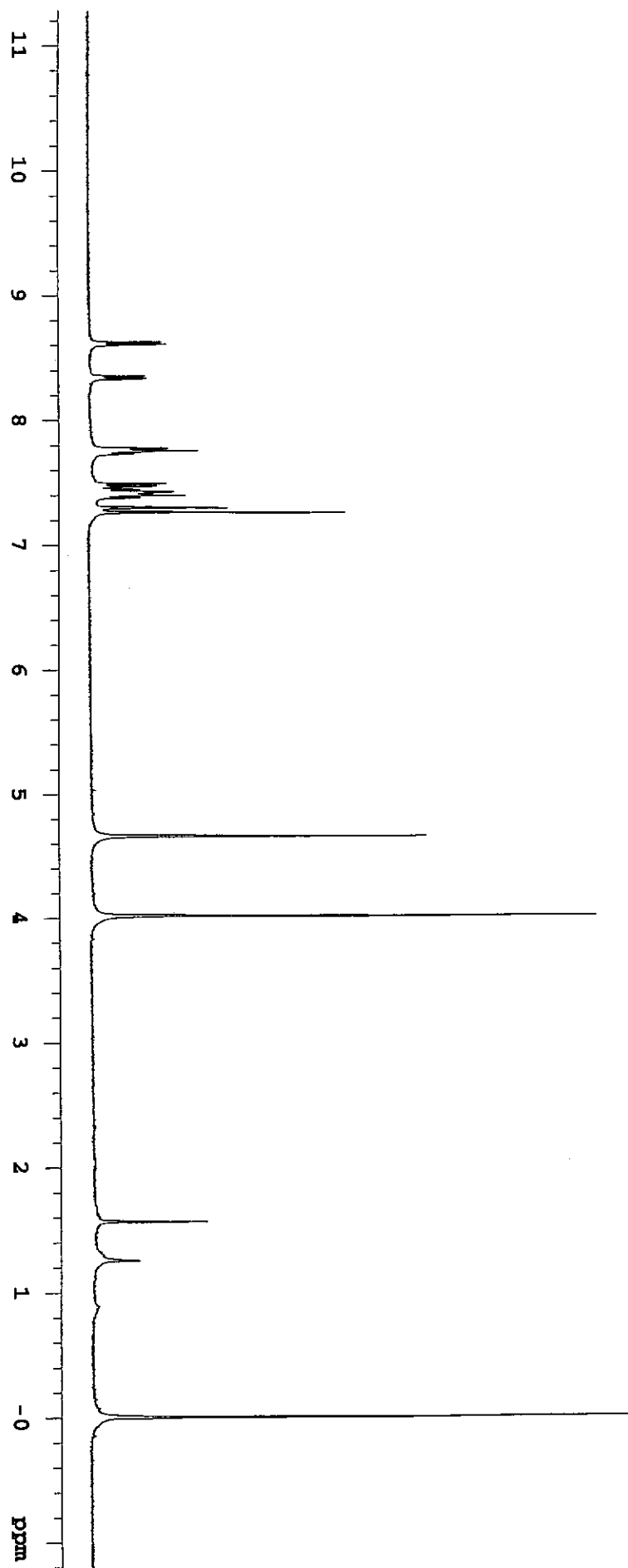
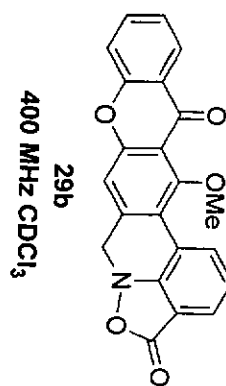
INDEX	FREQUENCY	PPM	HEIGHT
1	21613.250	215.000	-4.8
2	17539.029	174.471	10.1
3	16470.119	163.838	9.4
4	15846.778	157.637	9.4
5	15779.637	156.970	8.9
6	15544.645	154.632	12.0
7	15096.786	150.177	13.9
8	14983.867	149.054	7.4
9	13698.275	136.265	16.2
10	13599.853	135.286	14.8
11	13216.083	131.468	18.1
12	13145.890	130.770	14.3
13	12917.001	128.493	11.7
14	12670.564	126.042	18.2
15	12515.683	124.501	15.5
16	12454.646	123.894	12.6
17	12306.631	122.421	11.6
18	12272.298	122.080	12.9
19	11838.935	117.769	19.5
20	11433.802	113.739	8.0
21	11127.854	110.695	18.3
22	7973.003	79.312	7.9
23	7939.432	78.978	9.0
24	7906.625	78.652	9.2
25	6245.655	62.129	19.1
26	6079.329	60.475	16.6
27	5358.329	53.303	17.6
28	4034.589	40.134	122.8
29	4013.226	39.922	371.5
30	3992.626	39.717	722.9
31	3971.263	39.505	863.5
32	3950.663	39.300	718.0
33	3929.300	39.087	368.9
34	3908.700	38.882	119.8
35	11.486	0.114	5.3



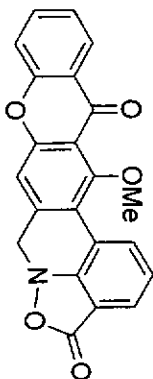
100 MHz DMSO-d₆



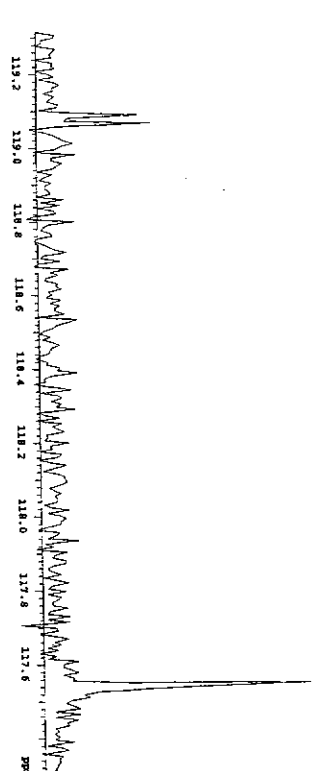
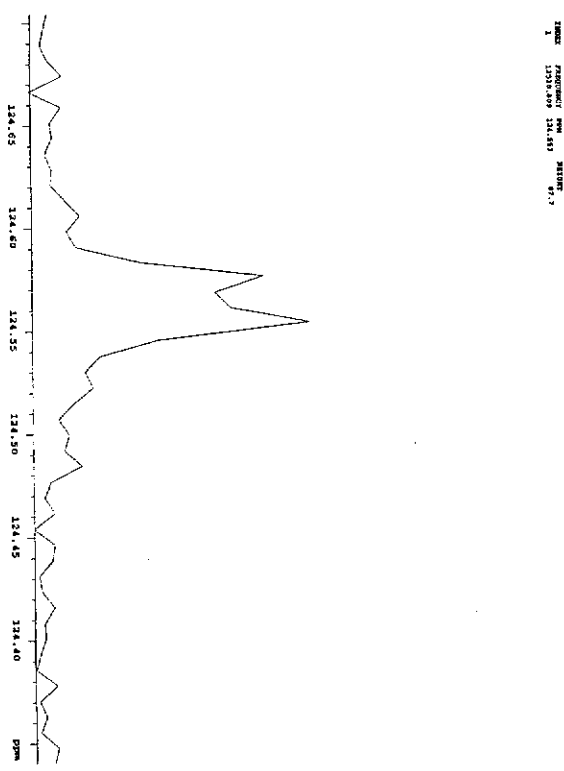
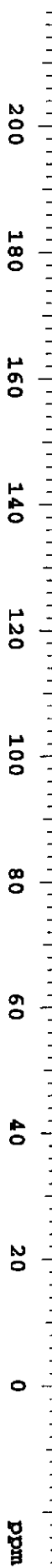


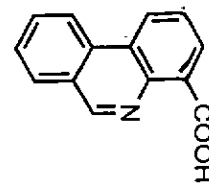


INDEX	FREQUENCY	PPM	HEIGHT
1	17646.392	175.540	7.0
2	16872.748	167.844	5.9
3	15972.452	158.888	7.2
4	15819.860	157.370	8.2
5	15756.534	156.741	6.7
6	15581.815	155.002	8.3
7	13987.986	139.148	13.3
8	13568.357	134.973	33.2
9	13285.297	132.158	29.7
10	12751.987	126.852	30.5
11	12703.157	126.367	33.6
12	12523.098	124.575	42.6
13	12330.831	122.663	11.6
14	11971.476	119.088	11.1
15	11815.831	117.540	35.3
16	11467.157	114.071	31.7
17	11192.491	111.339	10.0
18	7772.129	77.314	515.3
19	7740.084	76.996	534.3
20	7708.040	76.677	534.8
21	6217.974	61.854	19.0
22	5632.018	56.025	33.3
23	-2.462	-0.024	19.5



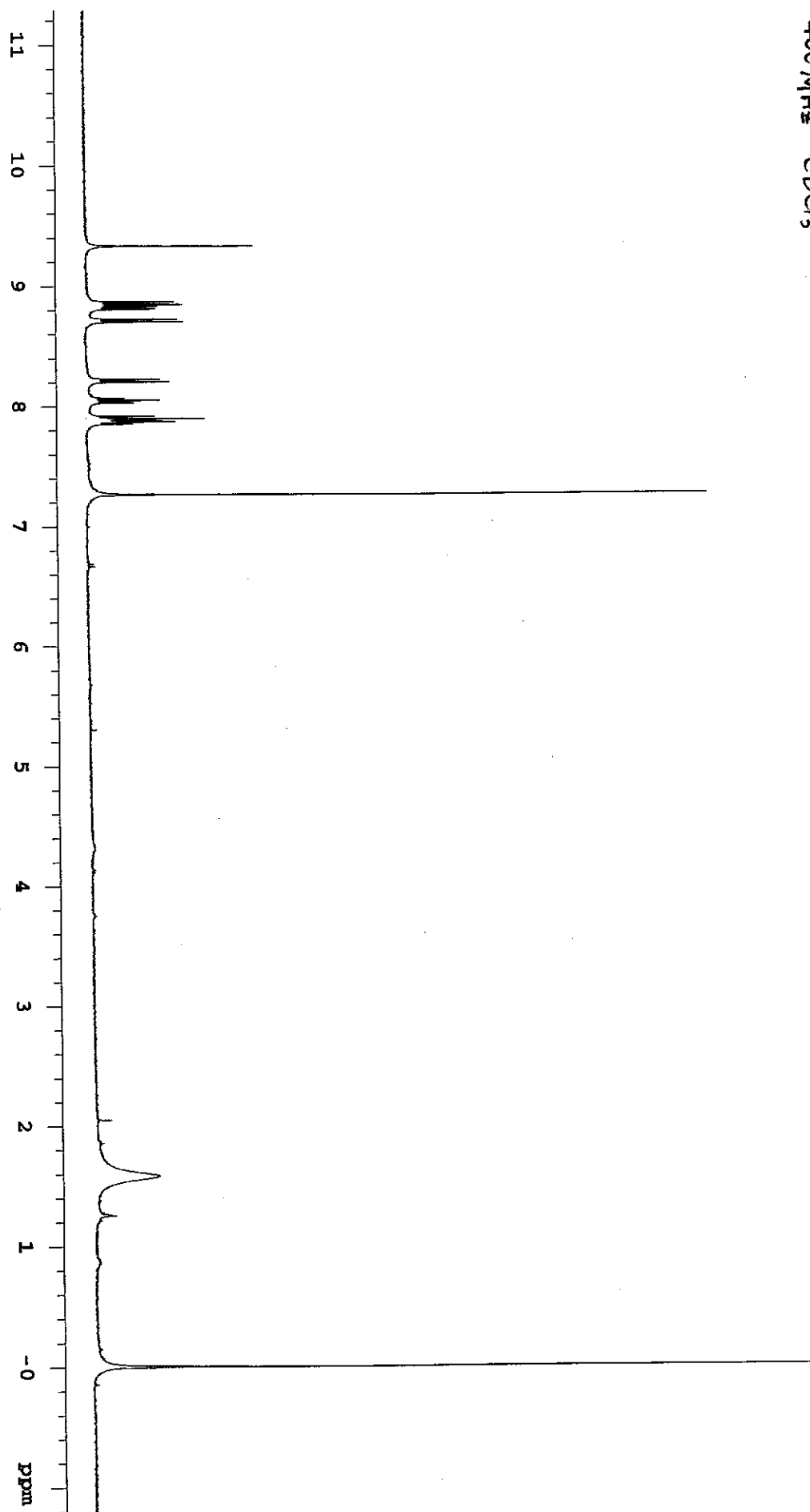
29b
100 MHz CDCl₃

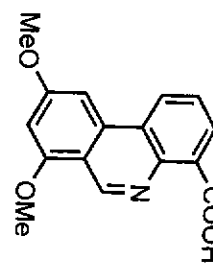




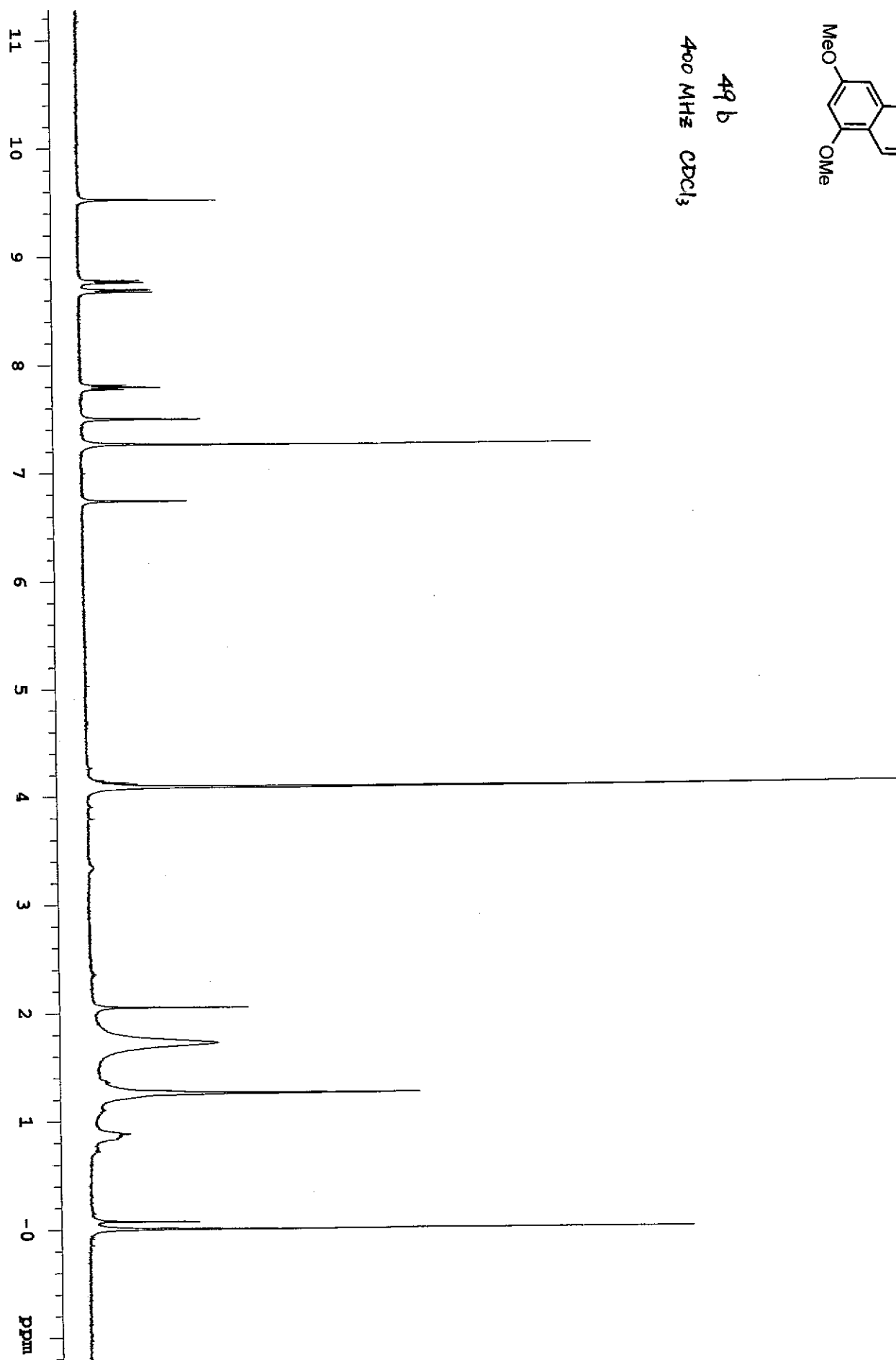
49 a

400 MHz CDCl₃

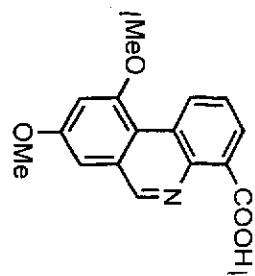




49b

400 MHz CDCl₃

Run-4-113-3



49c

400 MHz CDCl₃

