

Supporting Information

Exploration of Photochemical Reactions of *N*-Trimethylsilylmethyl-Substituted Uracil, Pyridone, and Pyrrolidone Derivatives

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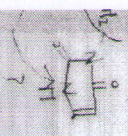
³*Basic Science Research Institute, Pukyong National University, Busan 608-735, Korea*

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New Mexico 87131, USA*

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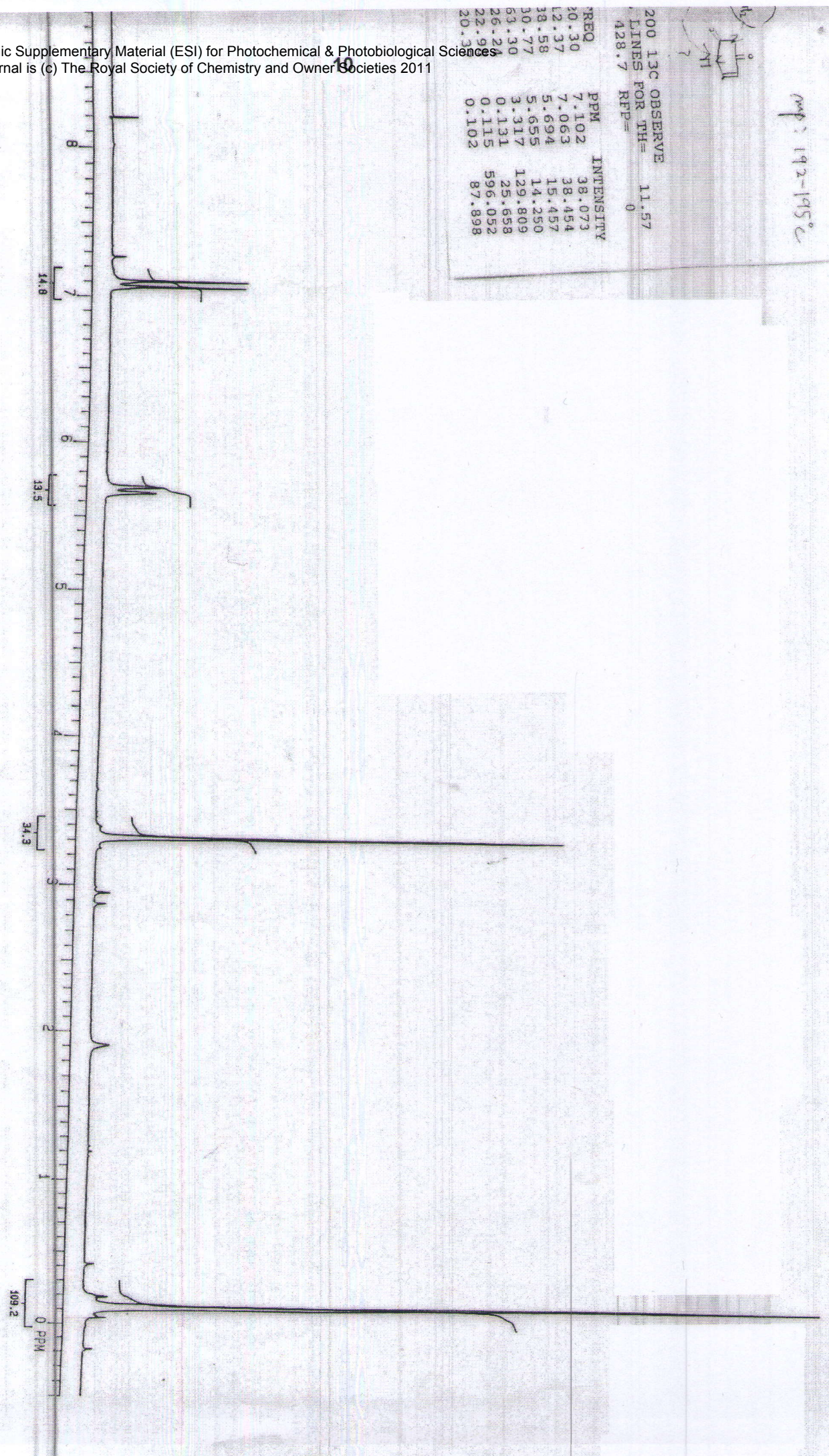
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¹H and ¹³C-NMR Spectra



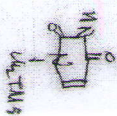
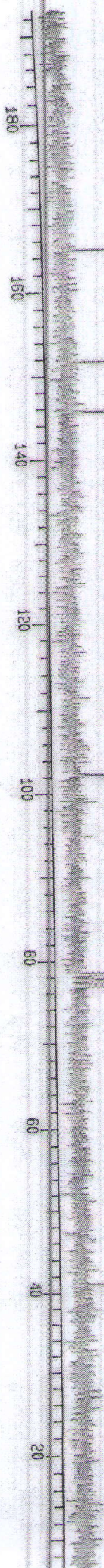
mp: 192-195°C

200 13C OBSERVE	11.57	
LINES FOR TH=	0	
428.7 RFP=	0	
FREQ	PPM	INTENSITY
20.30	7.102	38.073
12.37	7.063	38.454
38.58	5.694	15.457
30.77	5.655	14.250
63.30	3.317	129.809
26.27	0.131	25.658
22.93	0.115	596.052
20.30	0.102	87.898



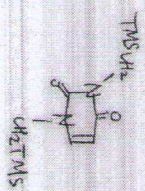
GEMINI-200 13C OBSERVE 15.92
SPECTRAL LINES FOR TH= 0
RFL= 862.8 RFP=

INDEX	FREQ	PPM	INTENSITY
01	8287.6	164.797	27.797
02	7623.0	151.582	30.275
03	7320.2	145.561	44.202
04	5140.0	102.208	41.732
05	3934.0	78.227	83.155
06	3901.8	77.586	86.577
07	3869.8	76.950	85.894
08	2055.4	40.872	30.151
09	-85.9	-1.707	131.266

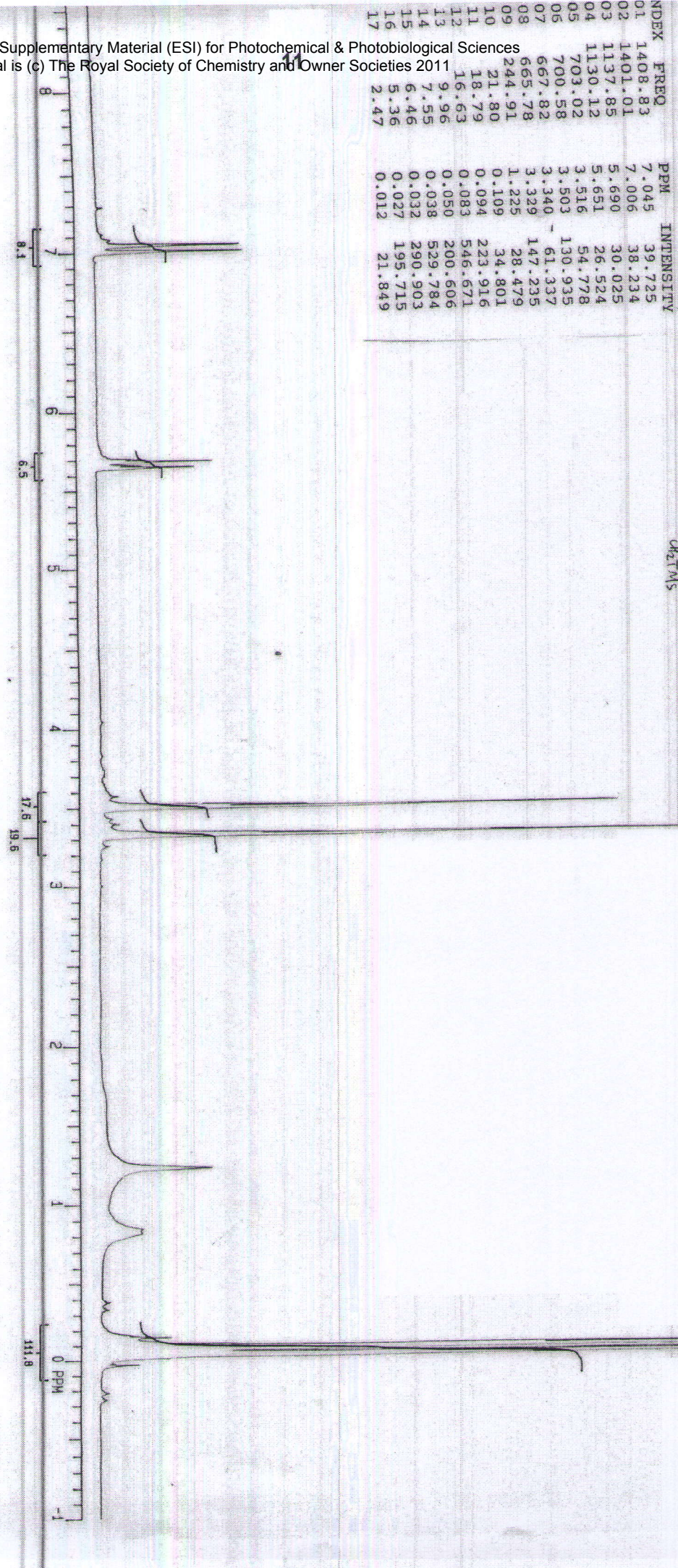


SEMNI-200 13C OBSERVE
SPECTRAL LINES FOR TH= 21.24
RFL= 428.7 RFB= 0

95.6



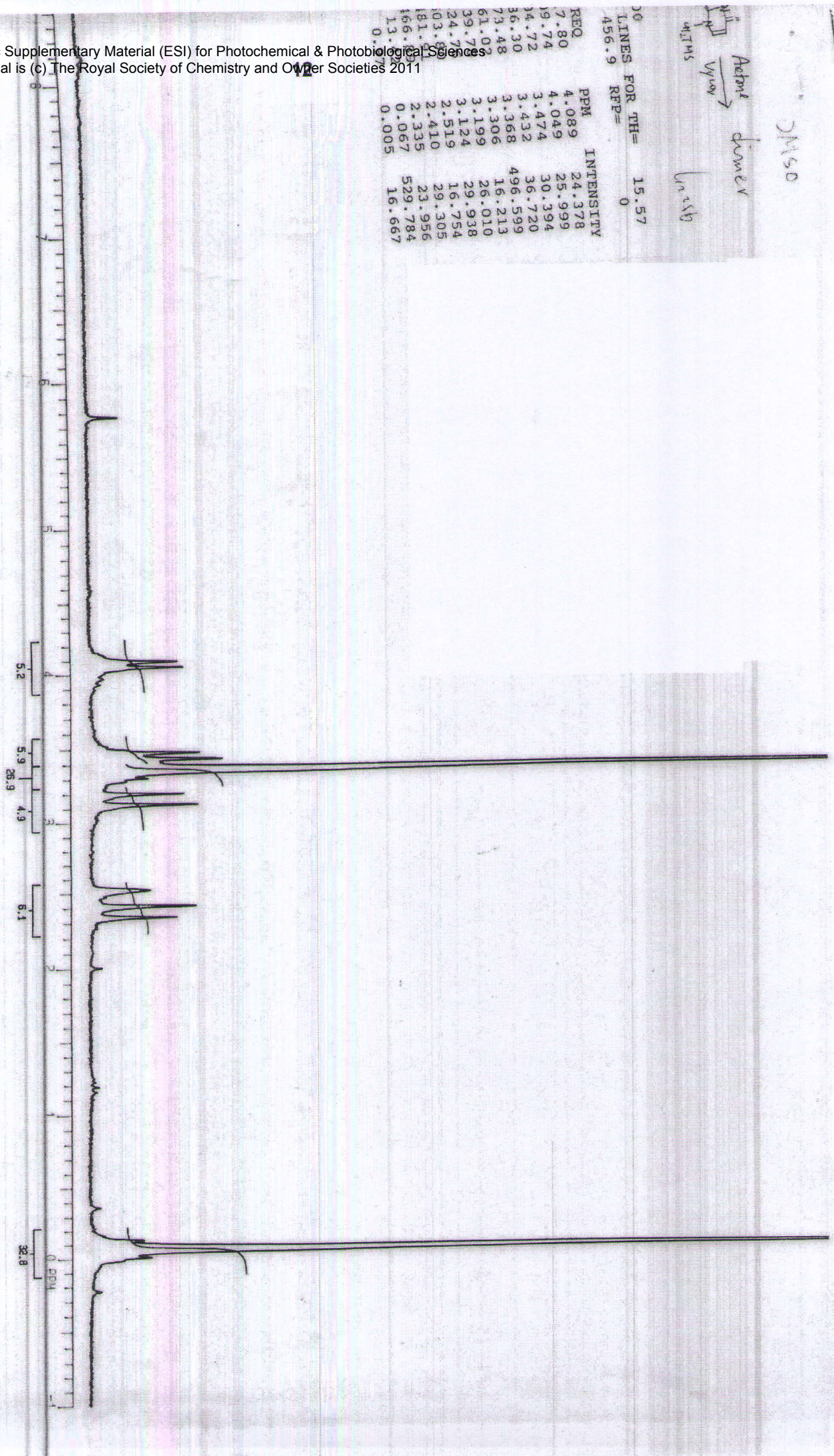
NDEX	FREQ	PPM	INTENSITY
01	1408.83	7.045	39.725
02	1401.01	7.006	38.234
03	1137.85	5.690	30.025
04	1130.12	5.651	26.524
05	703.02	3.516	54.778
06	700.58	3.503	130.935
07	667.82	3.340	61.337
08	665.78	3.329	147.235
09	244.91	1.225	28.479
10	21.80	0.109	34.801
11	18.79	0.094	223.916
12	16.63	0.083	546.671
13	9.96	0.050	200.606
14	7.55	0.038	529.784
15	6.46	0.032	290.903
16	5.36	0.027	195.715
17	2.47	0.012	21.849



MINI-200 13C OBSERVE 15.92
CENTRAL LINES FOR TH= 0
FL= 862.8 RFP=

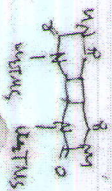
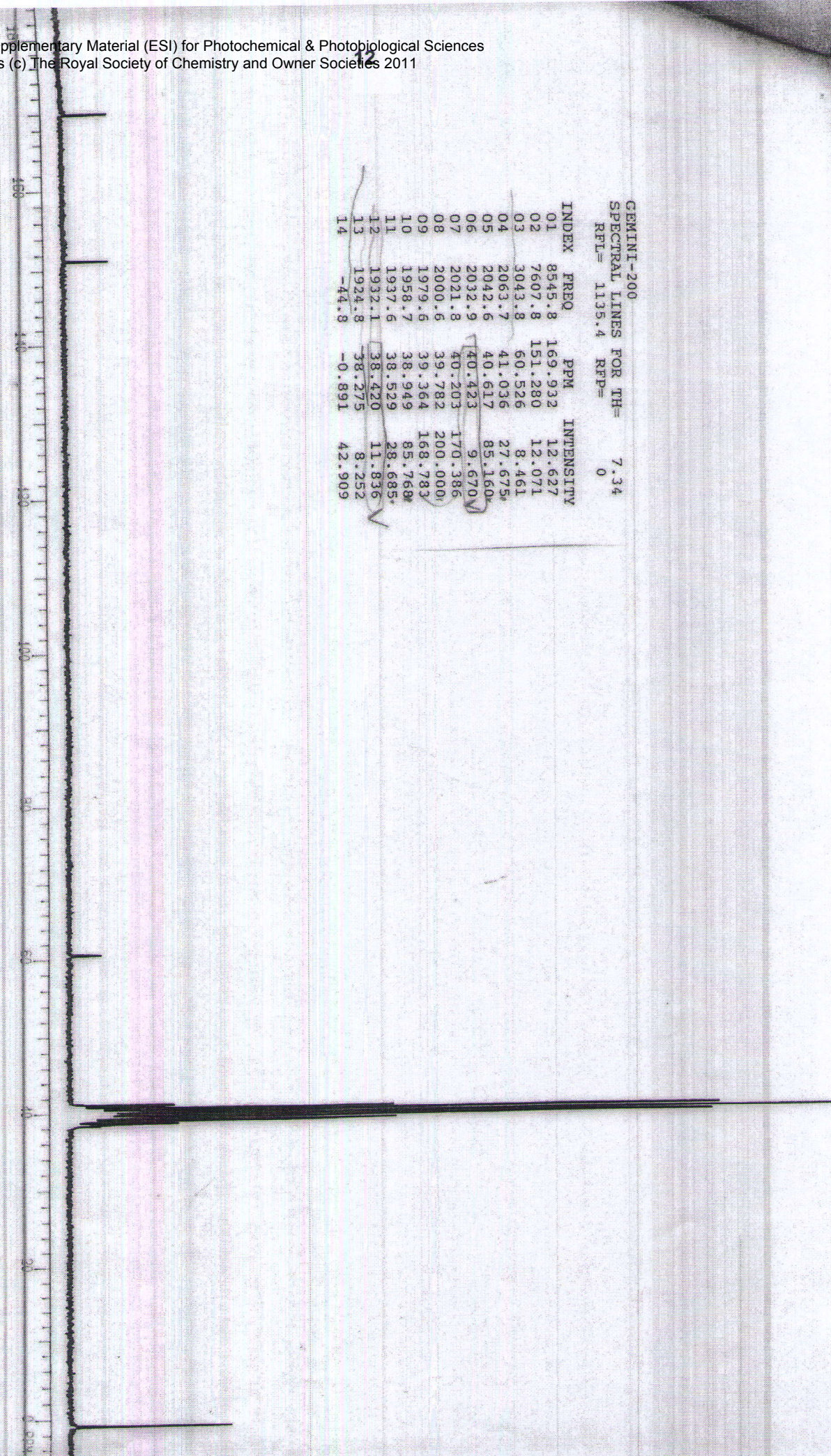
INDEX	FREQ	PPM	INTENSITY
1	8216.2	163.379	24.206
2	7634.9	151.819	19.169
3	7150.7	142.191	50.766
4	6984.8	101.111	34.374
5	6933.6	78.219	67.272
6	6901.7	77.584	68.660
7	6869.7	76.948	68.492
8	6814.6	41.849	27.635
9	6781.1	32.971	24.736
10	6711.5	-1.023	116.070
11	6733.7	-1.664	128.334





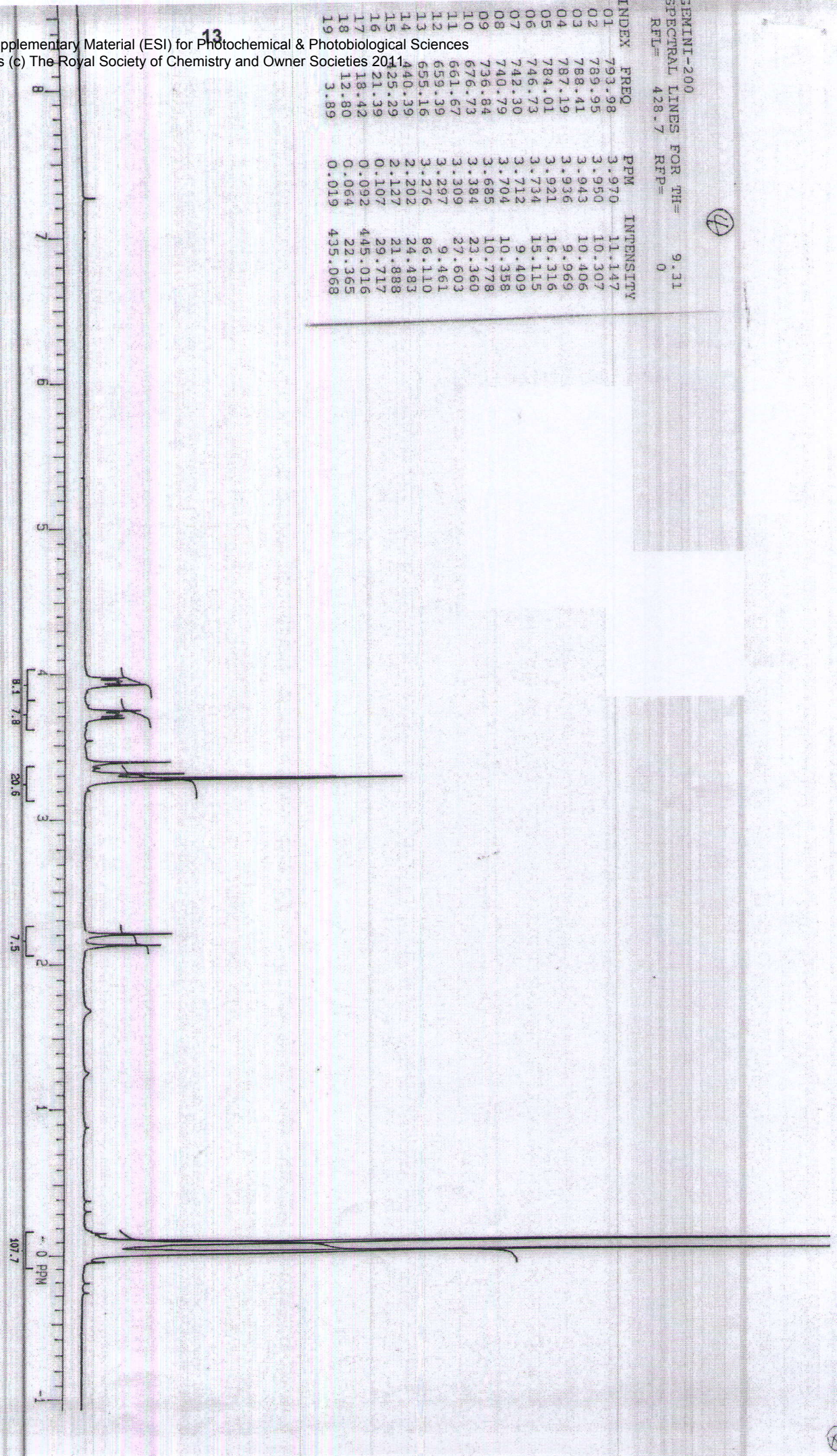
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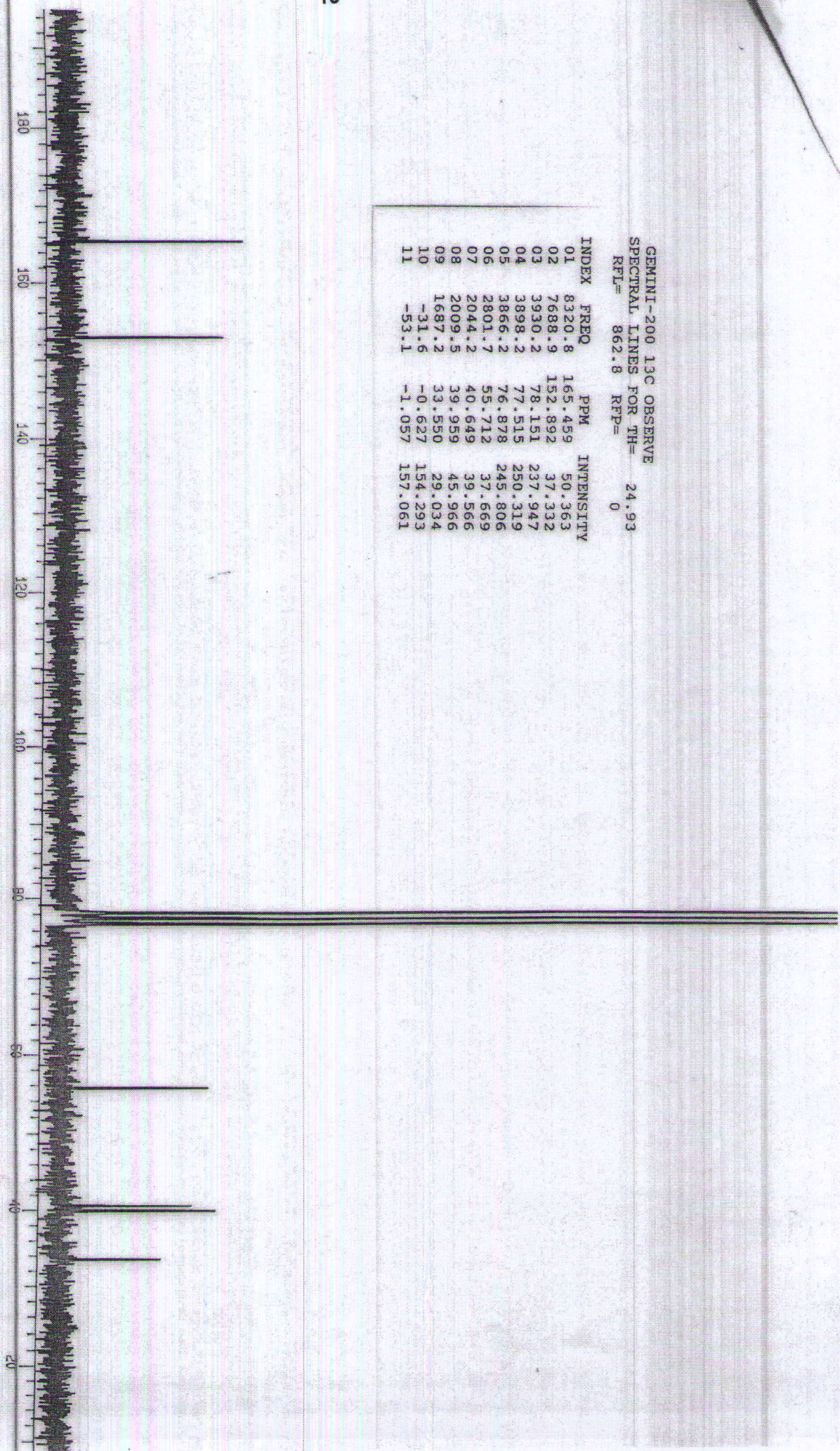
INDEX	FREQ	PPM	INTENSITY
01	8545.8	169.932	12.627
02	7607.8	151.280	12.071
03	3043.8	60.536	8.461
04	2063.7	41.036	27.675
05	2042.6	40.617	85.160
06	2032.9	40.423	9.670
07	2021.8	40.203	170.386
08	2000.6	39.782	200.000
09	1979.6	39.364	168.783
10	1958.7	38.949	85.768
11	1937.6	38.529	28.685
12	1932.1	38.420	11.836
13	1924.8	38.275	8.252
14	-44.9	-0.891	42.909



EMINI-200
SPECTRAL LINES FOR TH=
RFL= 428.7 RFP= 0 9.31

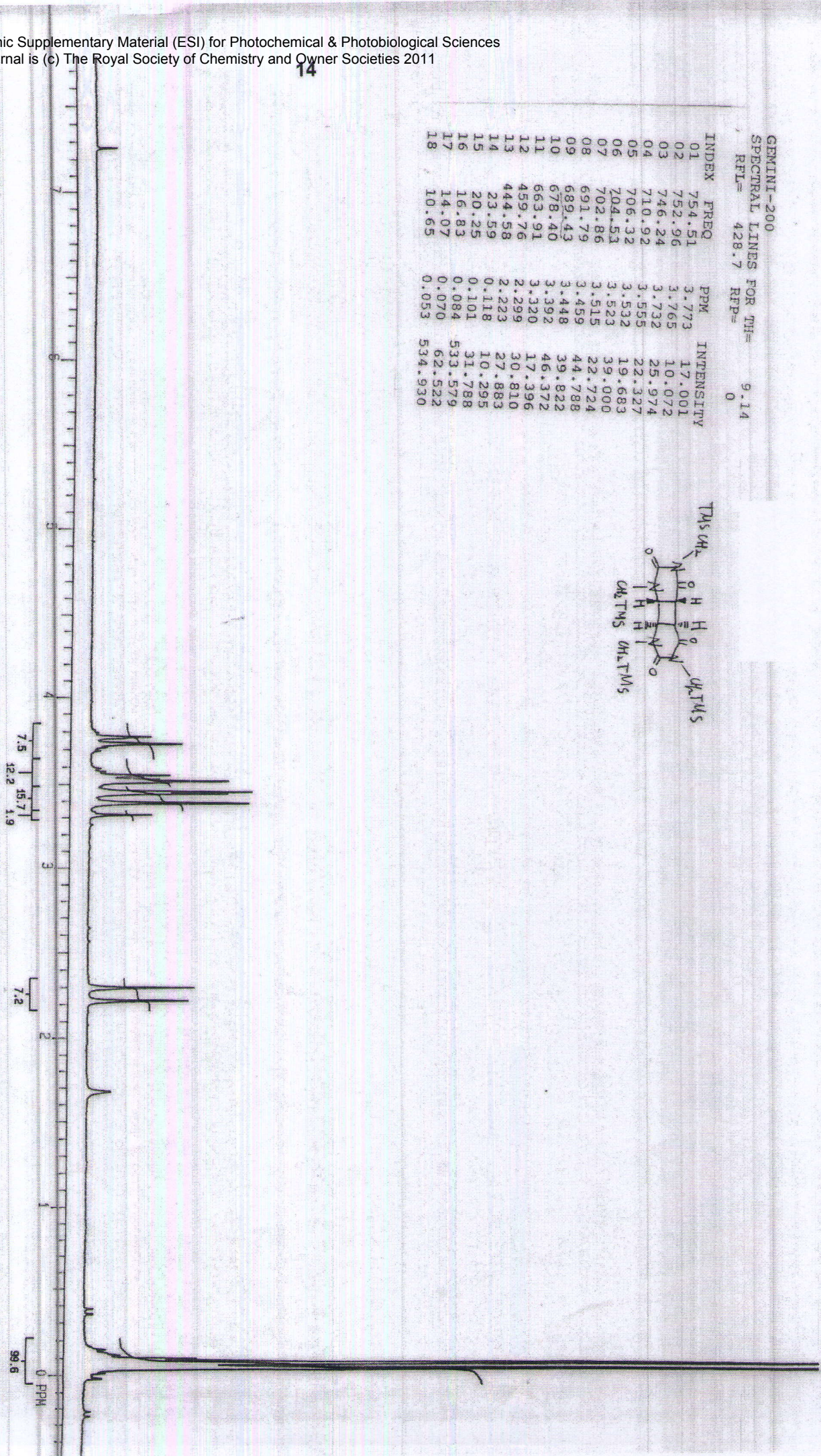
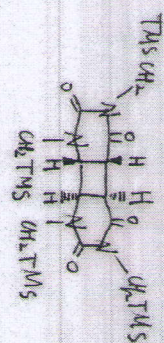
INDEX	FREQ	PPM	INTENSITY
01	793.98	3.970	11.147
02	789.95	3.950	10.307
03	788.41	3.943	10.406
04	787.19	3.936	9.969
05	784.01	3.921	16.316
06	746.73	3.734	15.115
07	742.30	3.712	9.409
08	740.79	3.704	10.358
09	736.64	3.685	10.778
10	676.73	3.384	23.360
11	661.67	3.309	27.603
12	659.39	3.297	9.461
13	655.16	3.276	86.110
14	440.39	2.202	24.483
15	225.29	2.127	21.888
16	21.39	0.107	29.717
17	18.42	0.092	445.016
18	12.80	0.064	22.365
19	3.89	0.019	435.068





GEMINI-200
 SPECTRAL LINES FOR TH= 9.14
 RFL= 428.7 RFP= 0

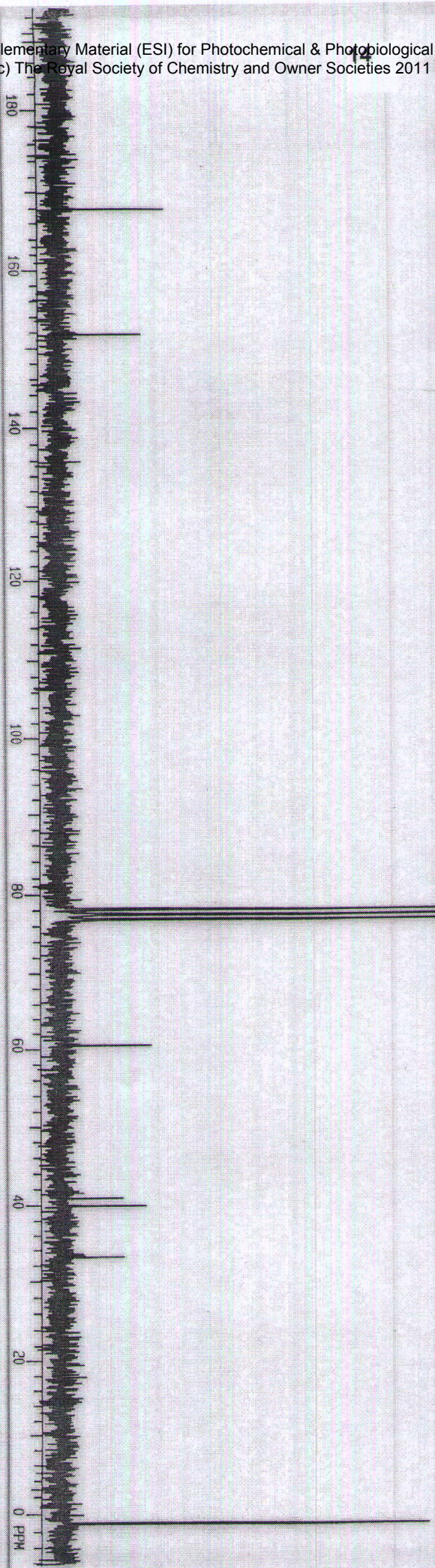
INDEX	FREQ	PPM	INTENSITY
01	754.51	3.773	17.001
02	752.96	3.765	10.072
03	746.24	3.732	25.974
04	710.92	3.555	22.327
05	706.32	3.532	19.683
06	704.53	3.523	39.000
07	702.86	3.515	22.724
08	691.79	3.459	44.788
09	689.43	3.448	39.822
10	678.40	3.392	46.372
11	663.91	3.320	17.396
12	459.76	2.299	30.810
13	444.58	2.223	27.883
14	23.59	0.118	10.295
15	20.25	0.101	31.788
16	16.83	0.084	533.579
17	14.07	0.070	62.522
18	10.65	0.053	534.930

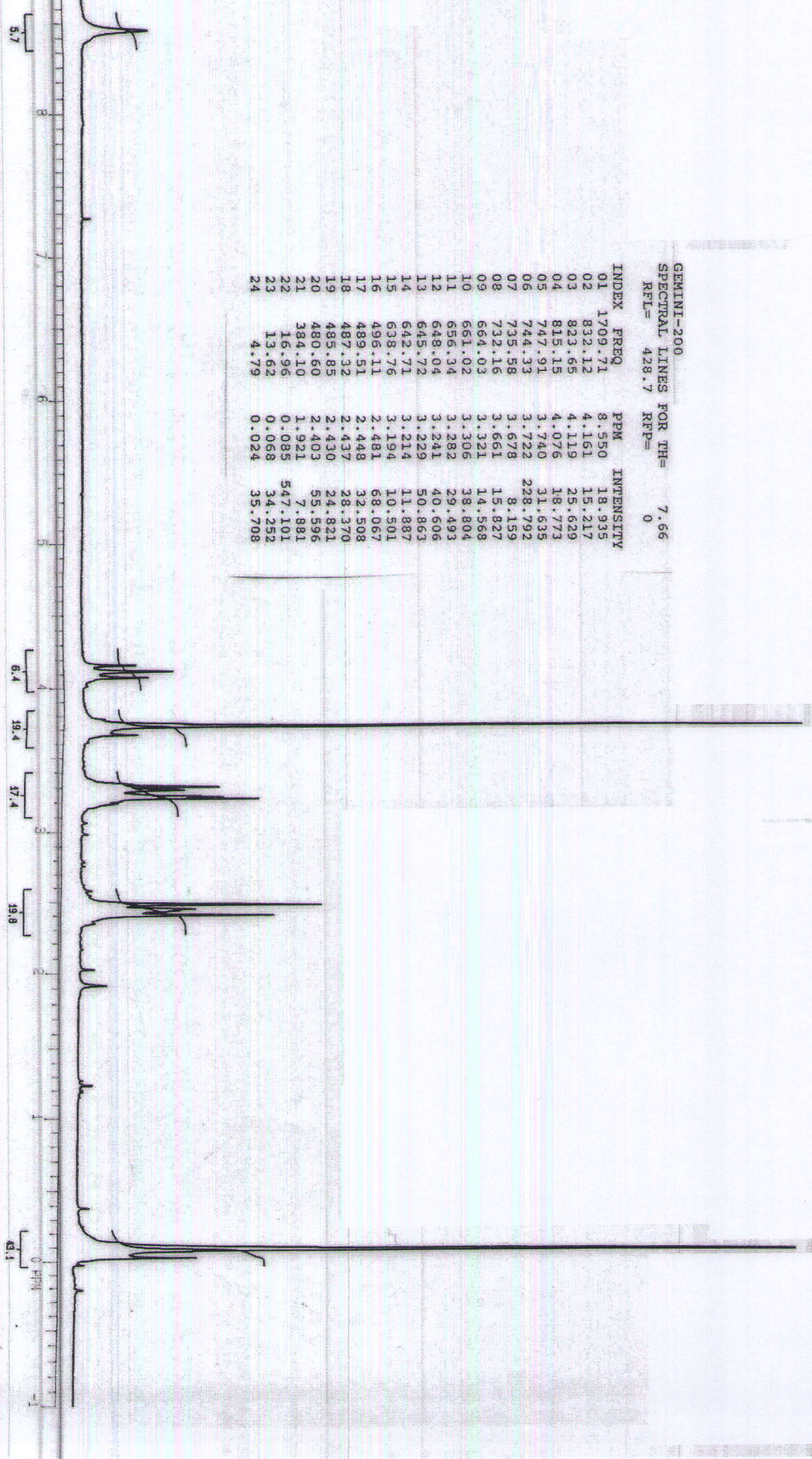


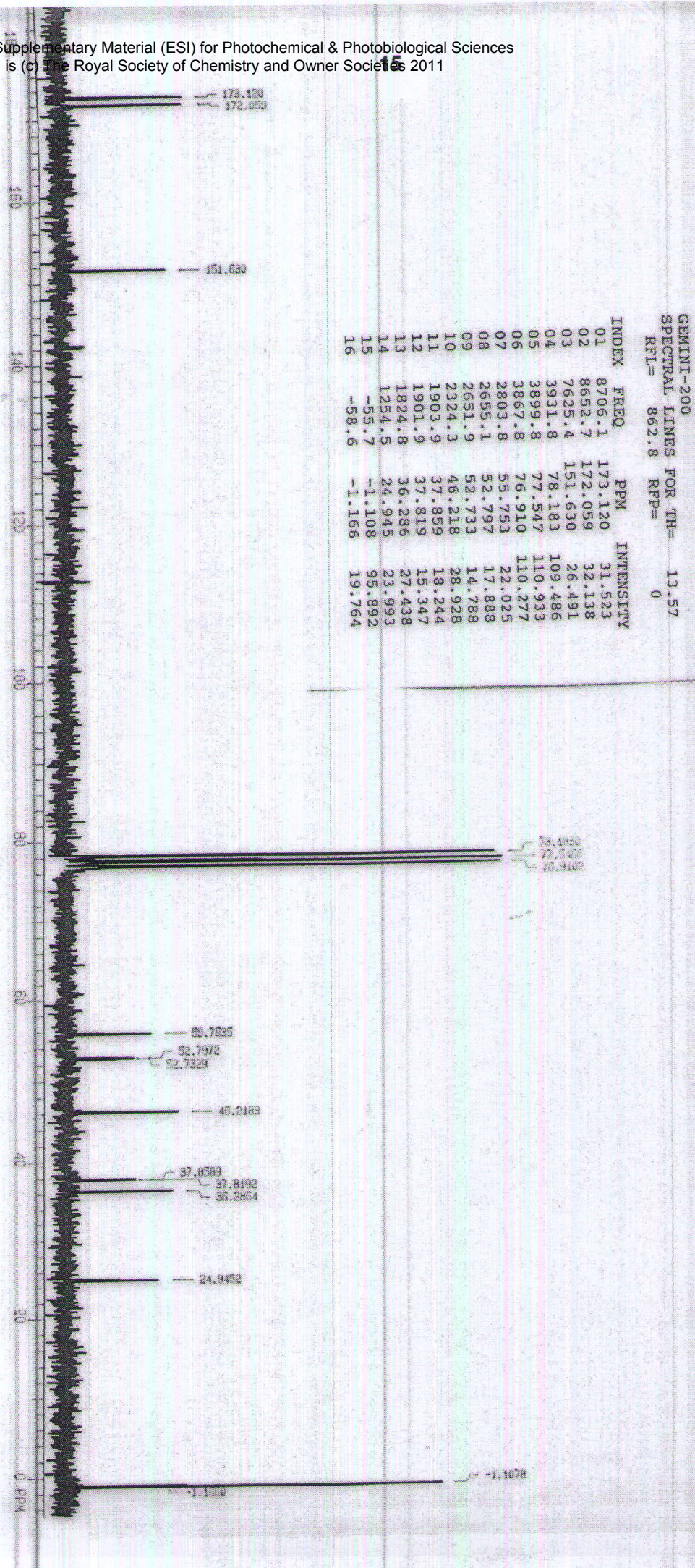
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SPECTRAL LINES FOR TH=
RFL= 862.8 RFP= 0

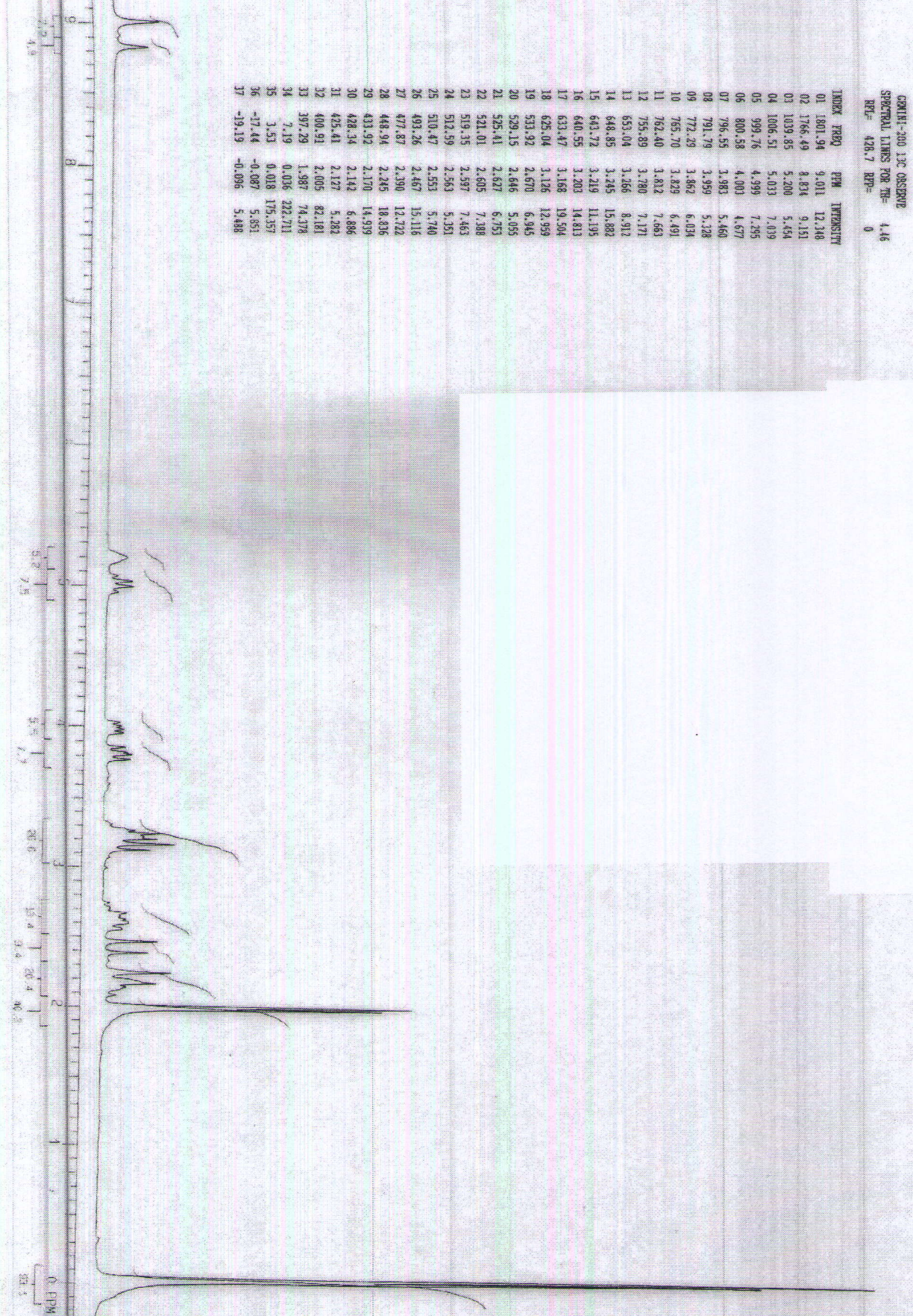
LC00 95222

INDEX	FREQ	PPM	INTENSITY
01	8448.2	167.993	28.176
02	7634.9	151.819	21.545
03	3929.6	78.140	193.138
04	3897.7	77.505	198.111
05	3865.7	76.870	196.524
06	3043.1	60.511	23.681
07	2054.7	40.857	16.064
008	2009.0	39.950	22.101
009	1667.7	33.163	16.419
010	-50.9	-1.012	89.486
011	-53.8	-1.071	96.911





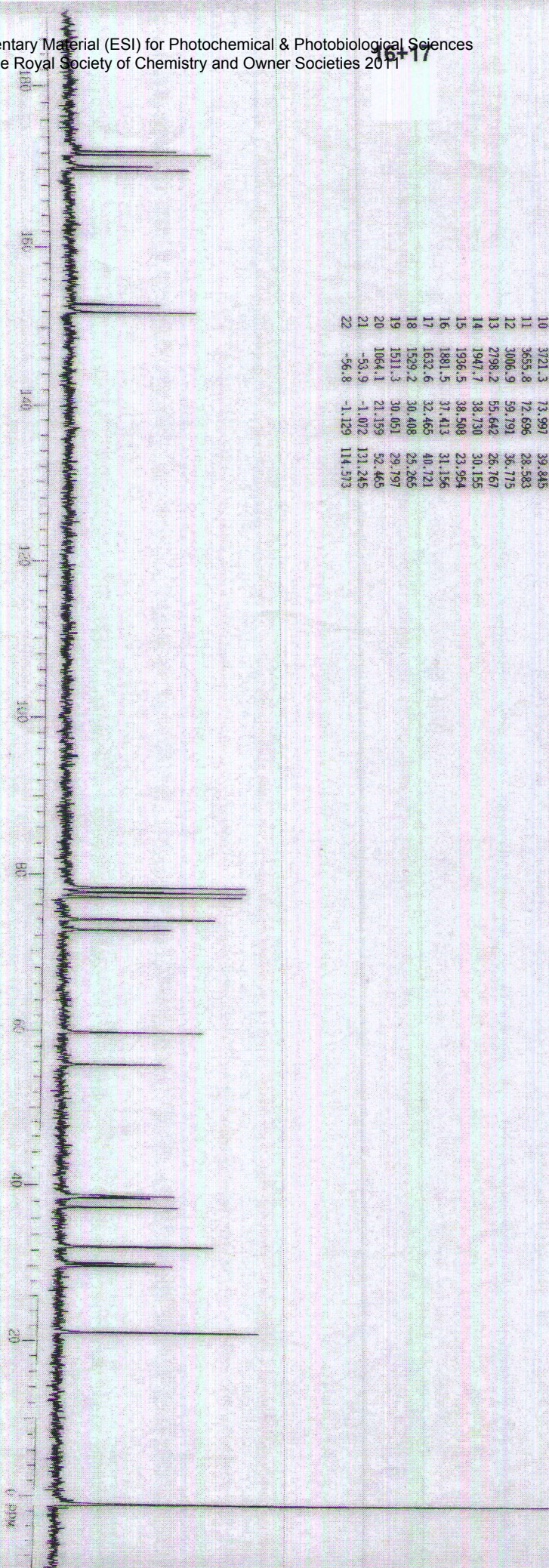




16+17

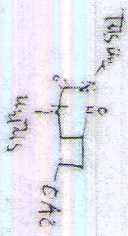
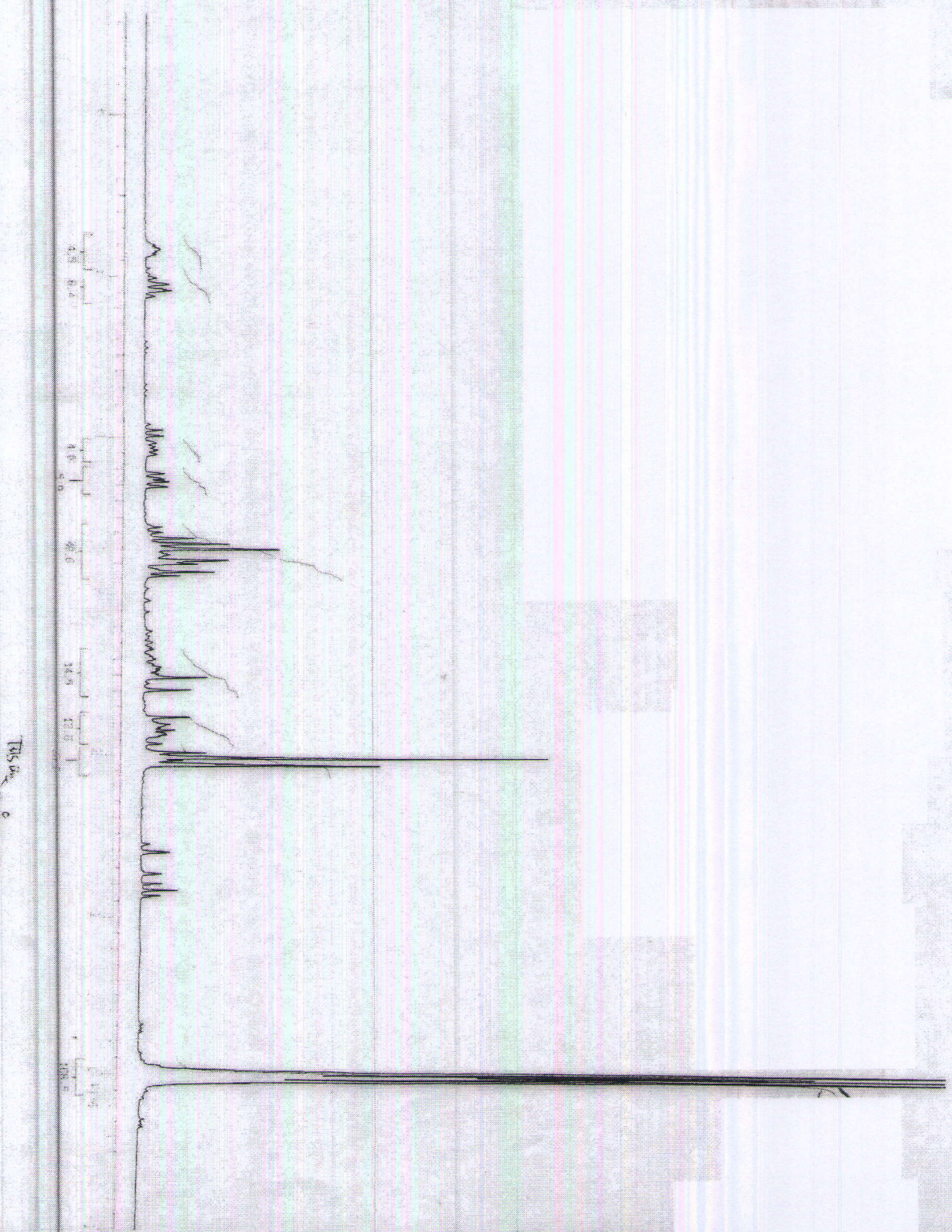
GEINUI-200 13C OSSEWE
SPECTRAL LINES FOR T₁= 11.17
RF1= 862.8 RF2= 0

INDEX	FREQ	PPM	INTENSITY
01	8662.9	172.260	28.320
02	8641.7	171.840	37.268
03	8588.3	170.380	22.028
04	8566.7	169.949	32.473
05	7692.8	152.971	23.601
06	7642.7	151.974	33.874
07	3937.2	79.291	47.415
08	3905.3	77.656	47.686
09	3873.0	77.015	46.985
10	3721.3	73.997	39.845
11	3655.8	72.696	28.583
12	3006.9	59.791	36.775
13	2798.2	55.642	26.767
14	1947.7	38.730	30.155
15	1936.5	38.508	23.954
16	1881.5	37.413	31.156
17	1632.6	32.465	40.121
18	1529.2	30.408	25.265
19	1511.3	30.051	29.797
20	1064.1	21.159	52.465
21	-53.9	-1.072	131.245
22	-56.8	-1.129	114.573



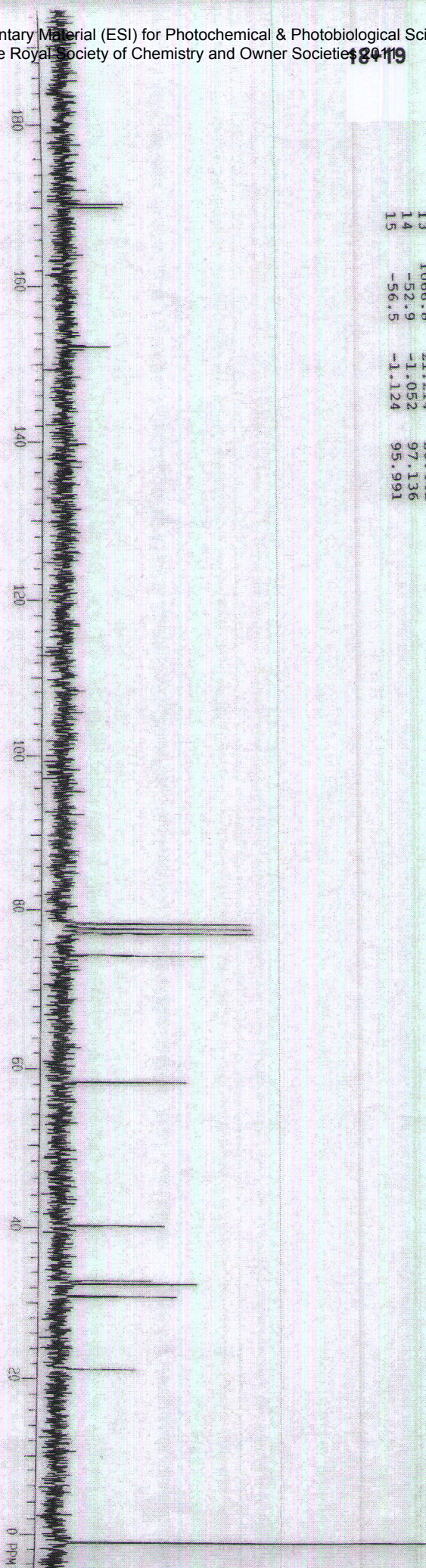
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 RFL= 428.7 RFP= 0

INDEX	FREQ	PPM	INTENSITY
01	1034.11	5.171	4.013
02	1032.81	5.165	3.987
03	990.97	4.955	6.418
04	989.67	4.949	6.227
05	983.11	4.916	7.152
06	809.29	4.047	5.051
07	802.04	4.011	5.097
08	754.51	3.773	5.472
09	748.12	3.741	5.438
10	744.45	3.723	6.671
11	738.02	3.691	6.399
12	686.66	3.434	5.028
13	679.99	3.400	5.152
14	672.38	3.362	13.216
15	665.42	3.327	22.160
16	658.09	3.291	35.021
17	650.48	3.253	6.971
18	644.13	3.221	21.866
19	639.21	3.196	14.218
20	628.87	3.145	18.592
21	623.74	3.119	9.672
22	510.64	2.554	5.044
23	506.73	2.534	4.651
24	505.06	2.526	4.019
25	501.23	2.506	4.385
26	...	2.485	16.993
27	...	2.409	12.789
28	...	2.236	12.490
29	...	2.205	3.998
30	338.64	2.193	7.396
31	336.52	2.183	6.065
32	334.37	2.172	4.931
33	331.92	2.160	8.977
34	226.23	2.131	6.597
35	223.87	2.120	4.907
36	114.71	2.120	5.592
37	97.94	2.074	16.824
38	97.94	1.990	107.054
39	94.16	1.971	10.918
40	89.92	1.950	26.274
41	88.01	1.940	63.459
42	77.76	1.940	7.686
43	53.05	1.265	5.622
44	40.84	1.204	5.729
45	33.80	1.169	10.405
46	26.56	1.133	5.344
47	9.67	0.048	6.042
48	3.08	0.015	329.559
49	-0.42	-0.002	173.542
50	-2.78	-0.014	212.523
51	-6.45	-0.032	324.195
52	-9.74	-0.049	32.855
53	-12.23	-0.061	9.812

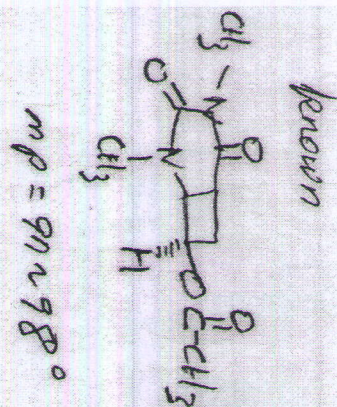
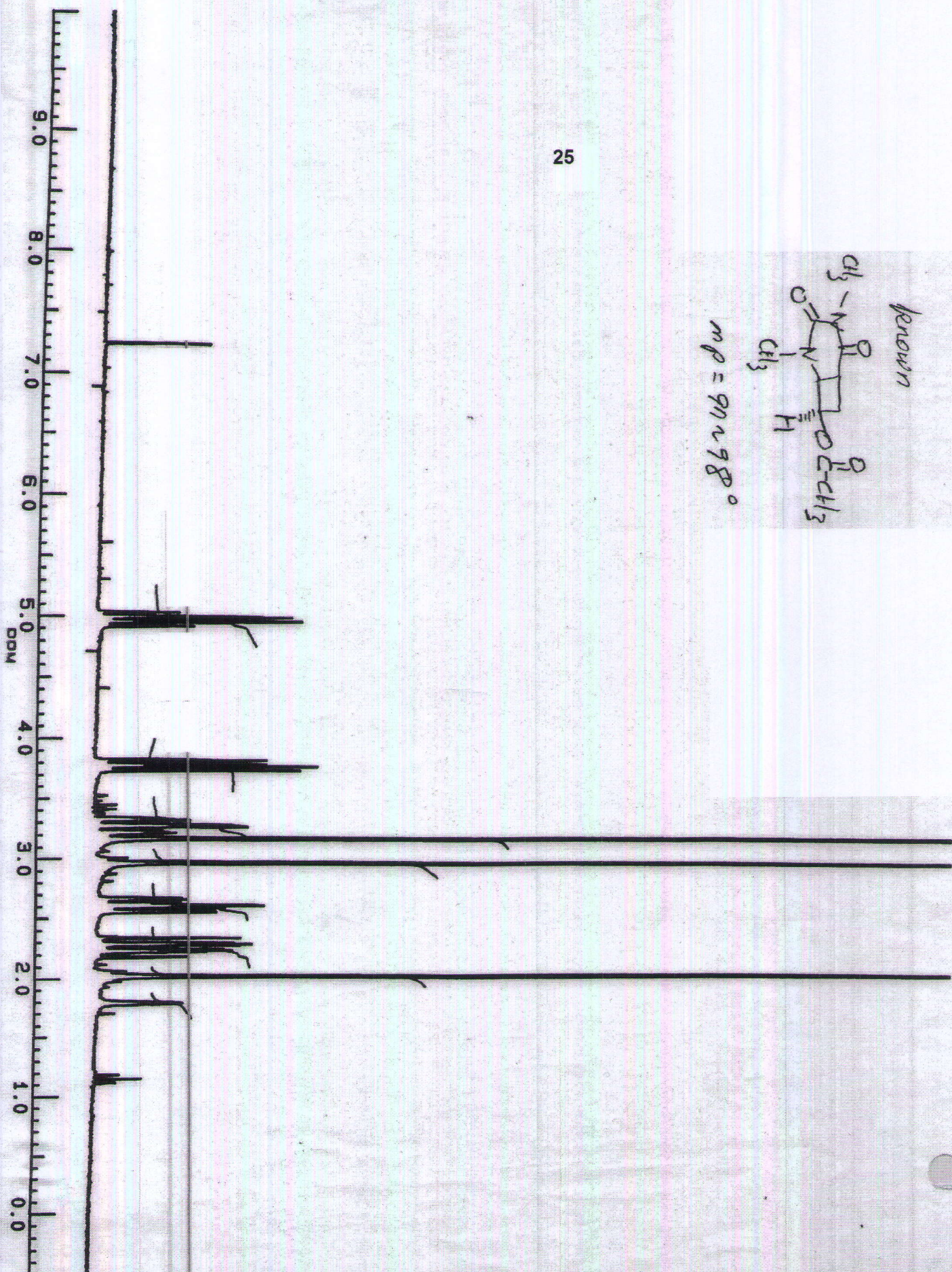


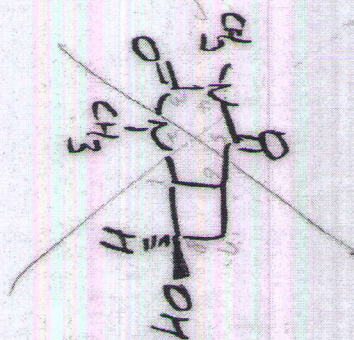
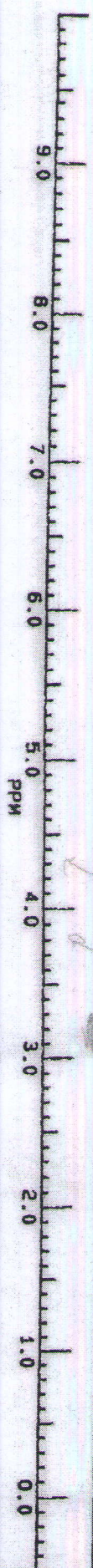
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RFL= 862.8 RFP= 0

INDEX	FREQ	PPM	INTENSITY
01	8570.4	170.422	16.054
02	8549.7	170.009	14.610
03	7662.9	152.377	12.370
04	3929.6	78.140	49.002
05	3897.7	77.505	49.357
06	3865.8	76.871	49.779
07	3732.0	74.211	37.250
08	2930.8	58.278	33.126
09	2020.7	40.181	27.781
10	1652.1	32.852	24.365
11	1632.5	32.463	36.400
12	1553.5	30.892	30.874
13	1066.8	21.214	20.442
14	-52.9	-1.052	97.136
15	-56.5	-1.124	95.991



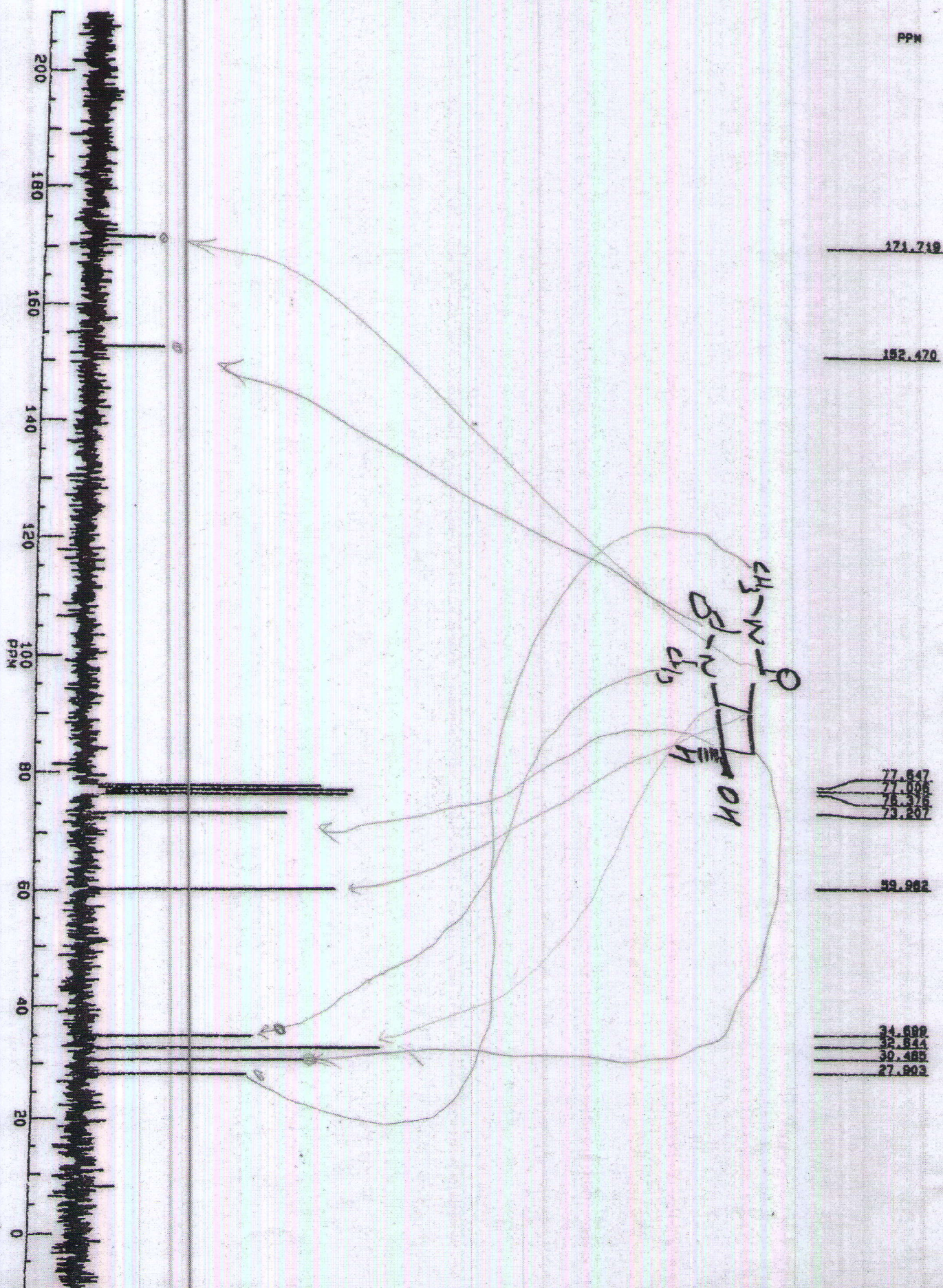
25





JP-3 200MHZ

3H₂O



PPM

171.719

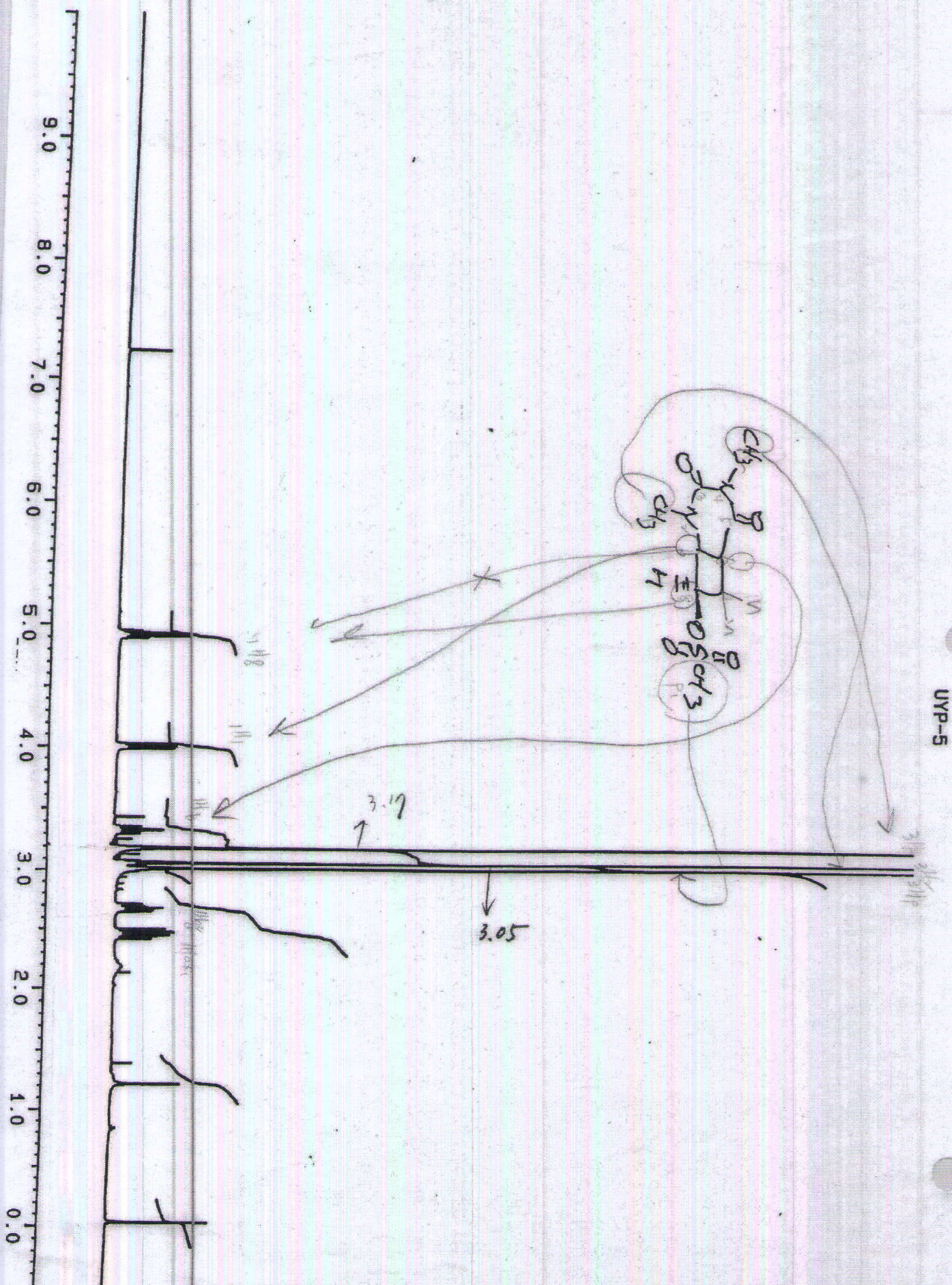
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UVP-3

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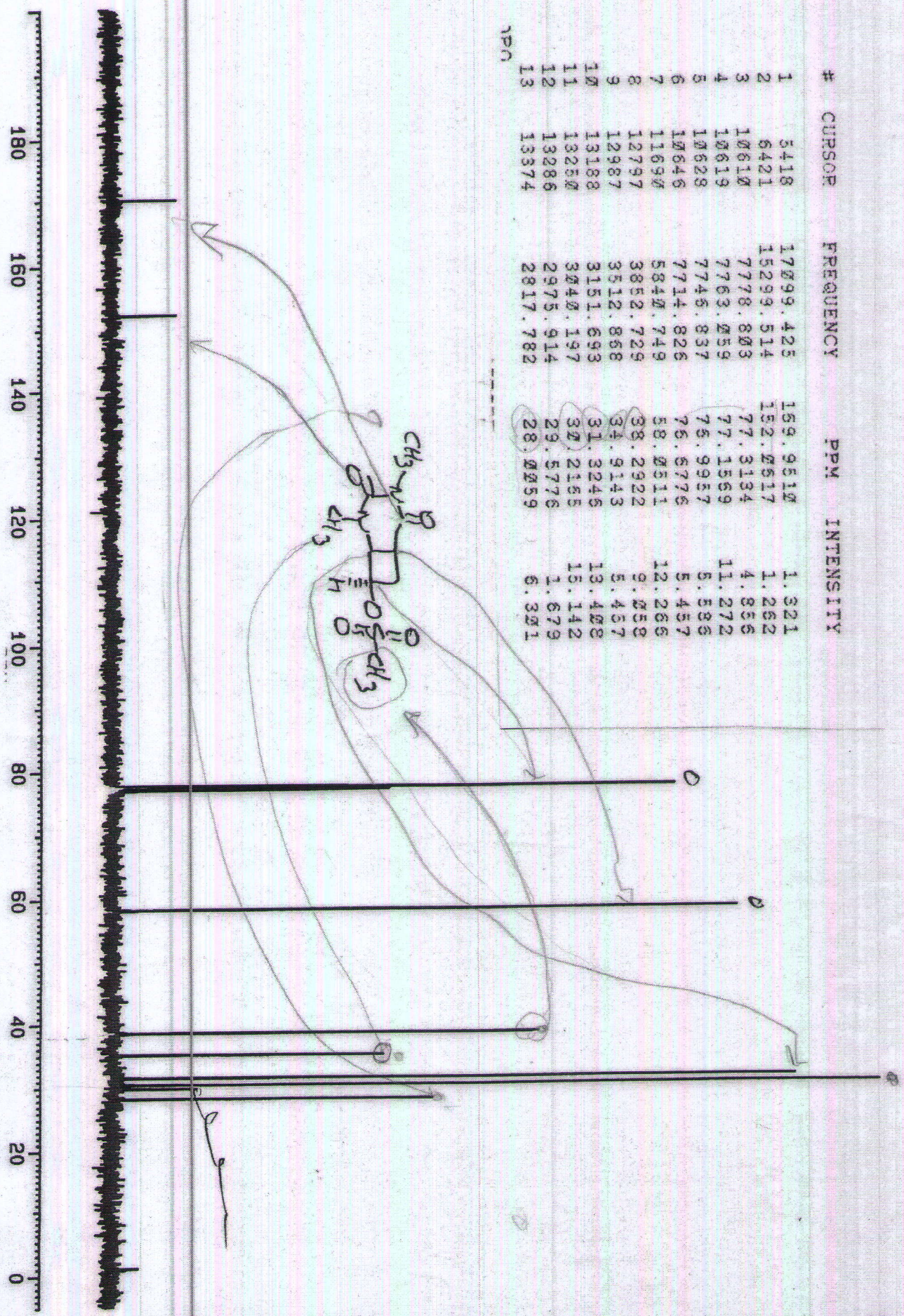
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34.892
32.844
30.483
27.903

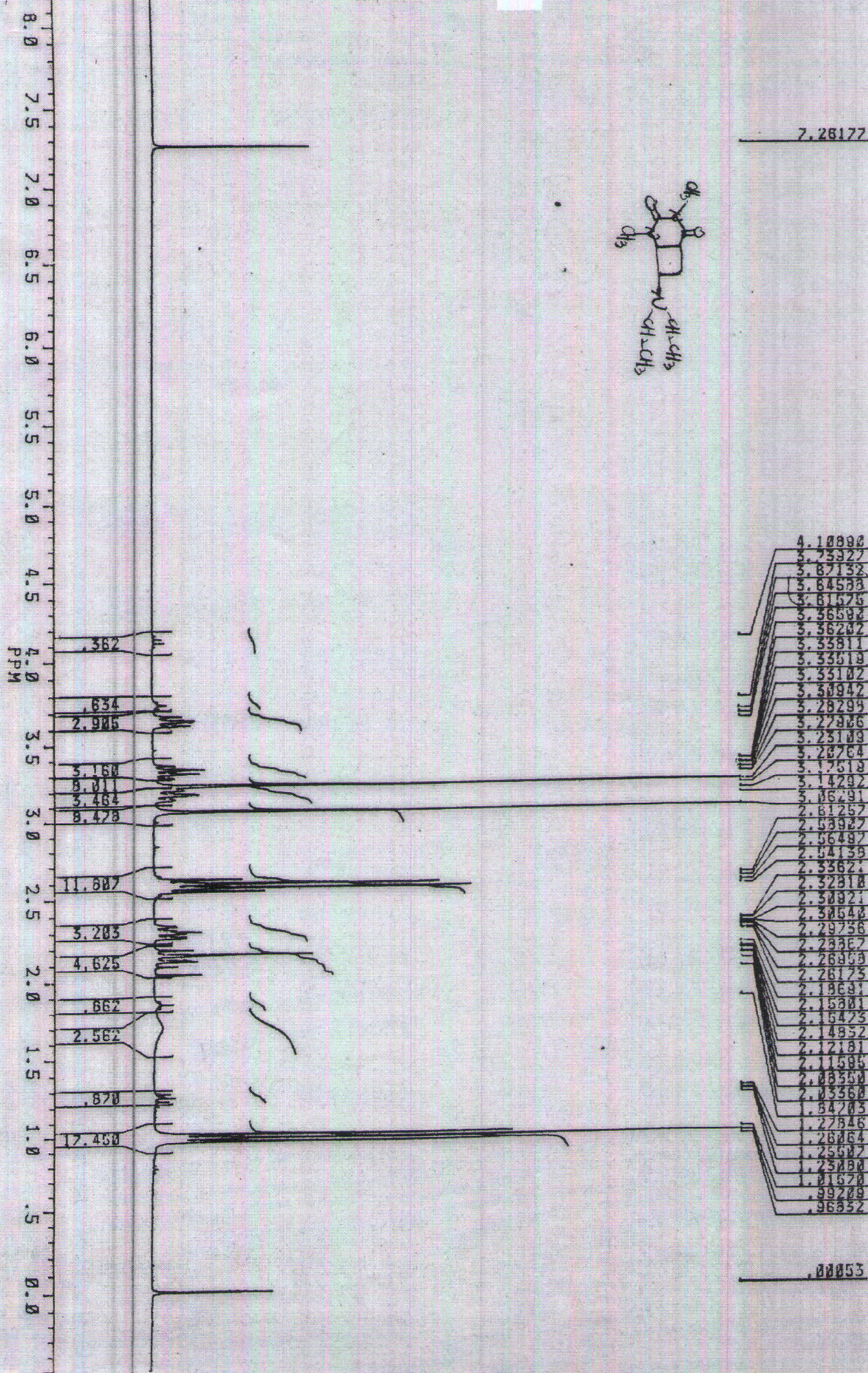


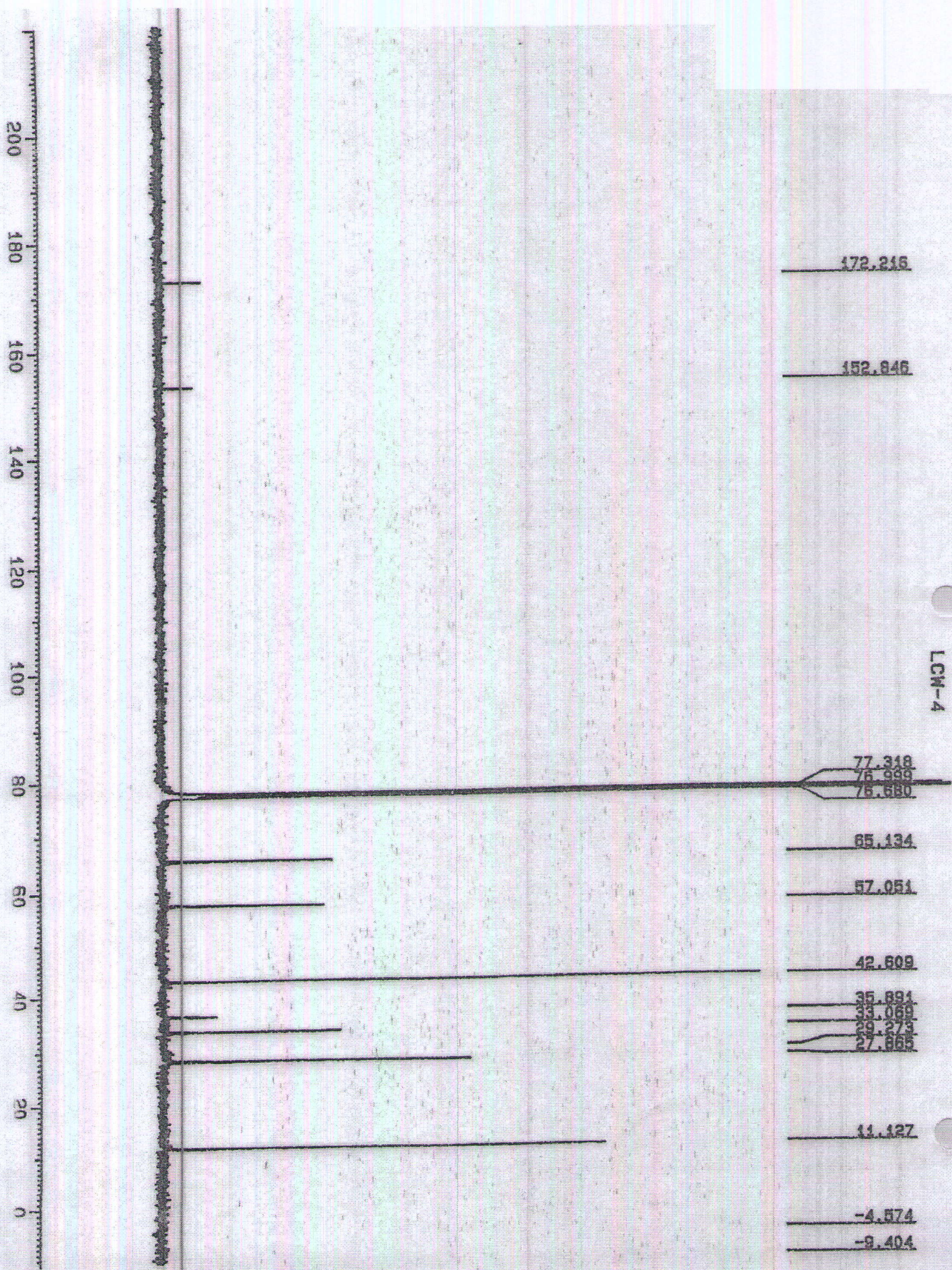
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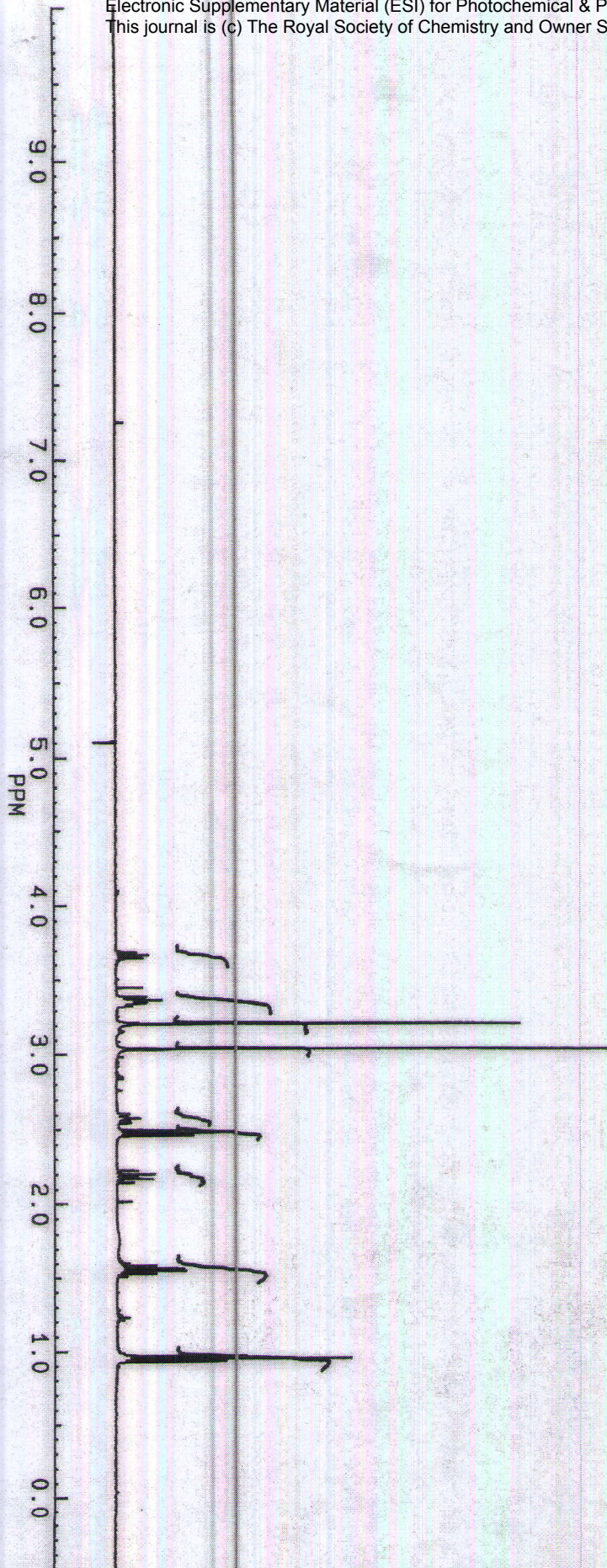
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1	5418	17099.425	159.9612	1.321
2	6421	15299.514	152.2617	1.262
3	10612	7778.803	77.3134	4.856
4	10619	7769.059	77.1569	11.272
5	10628	7745.837	75.9957	5.586
6	10646	7714.826	75.6776	5.457
7	11690	5840.749	58.0511	12.266
8	12797	3852.729	38.2922	9.258
9	12987	3512.868	34.9143	5.467
10	13188	3151.693	31.3246	13.422
11	13250	3040.197	30.2155	15.142
12	13286	2975.914	29.5776	1.679
13	13374	2817.782	28.0059	6.321

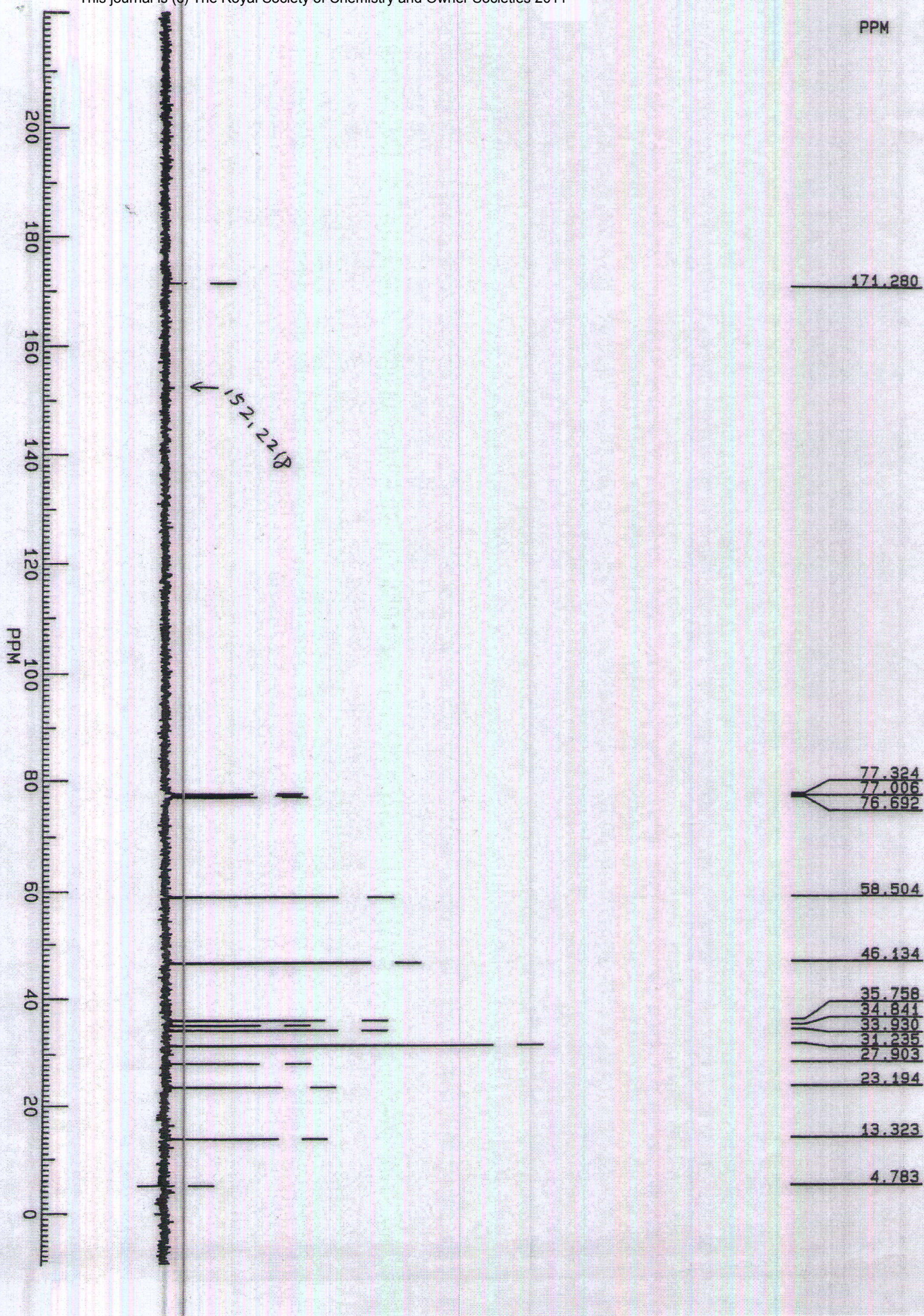


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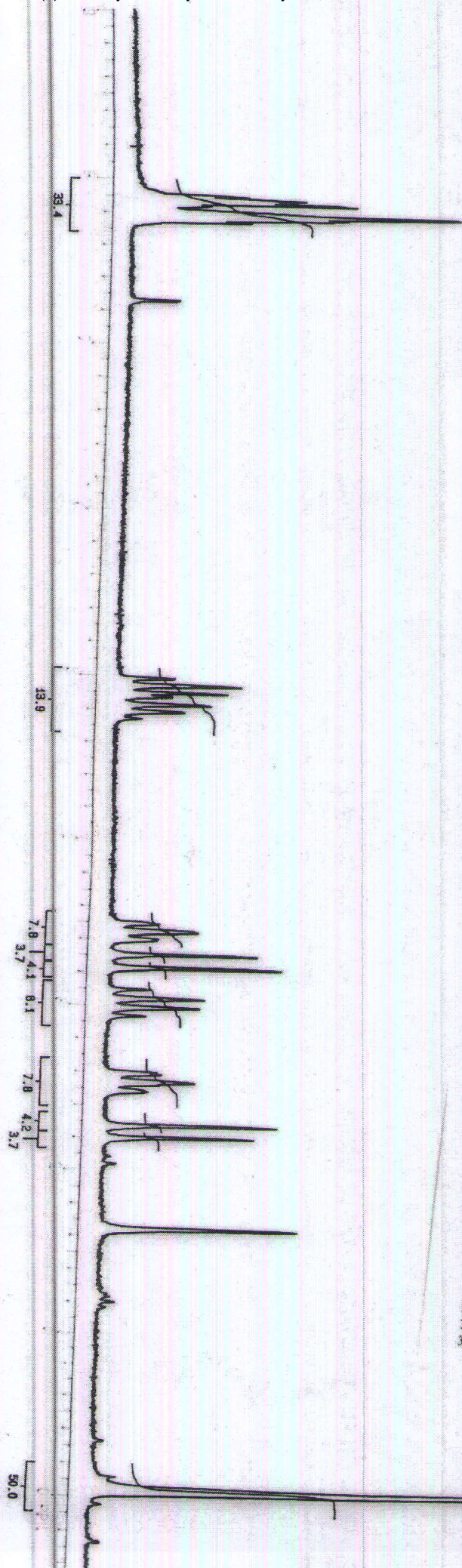








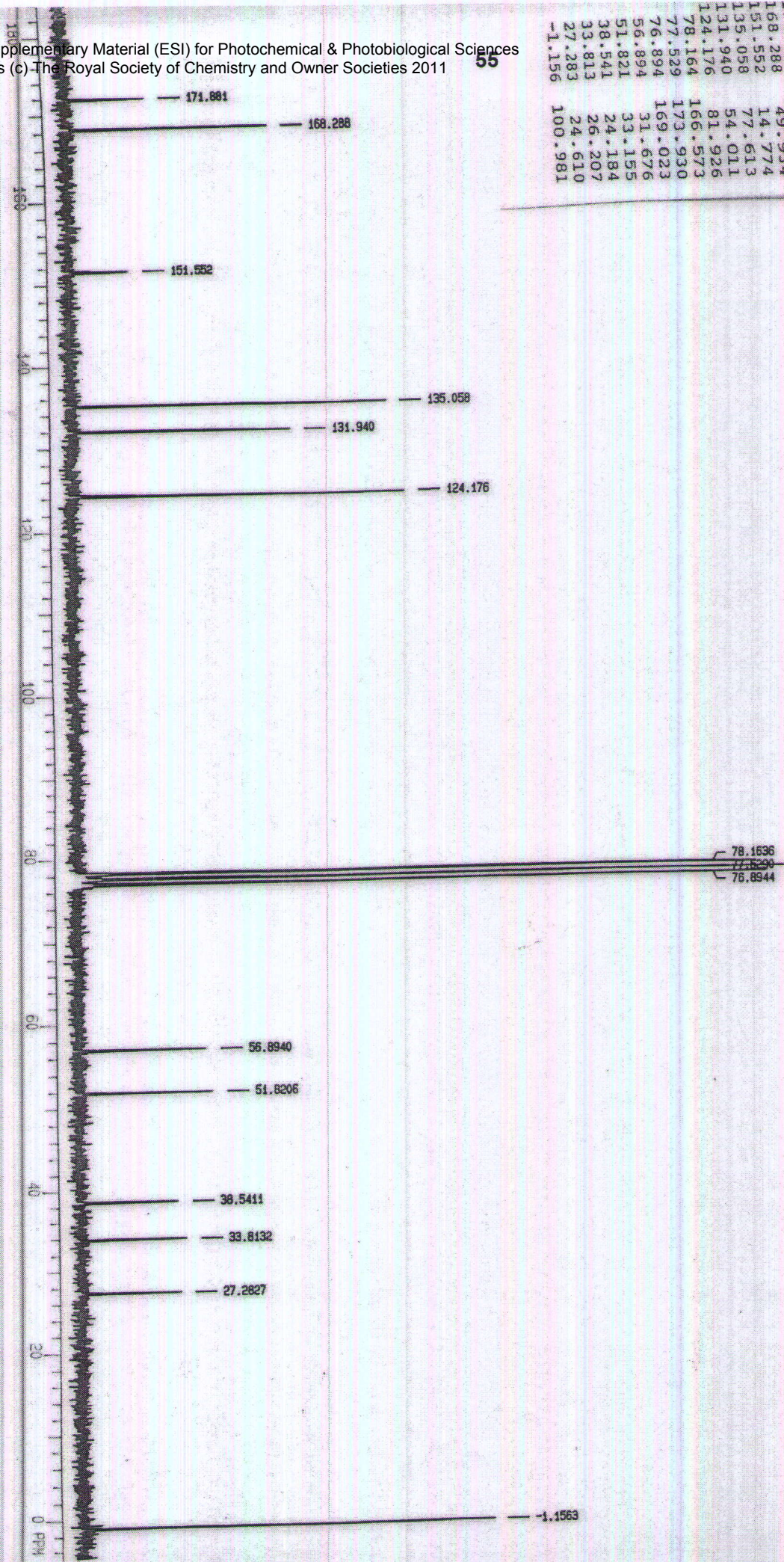
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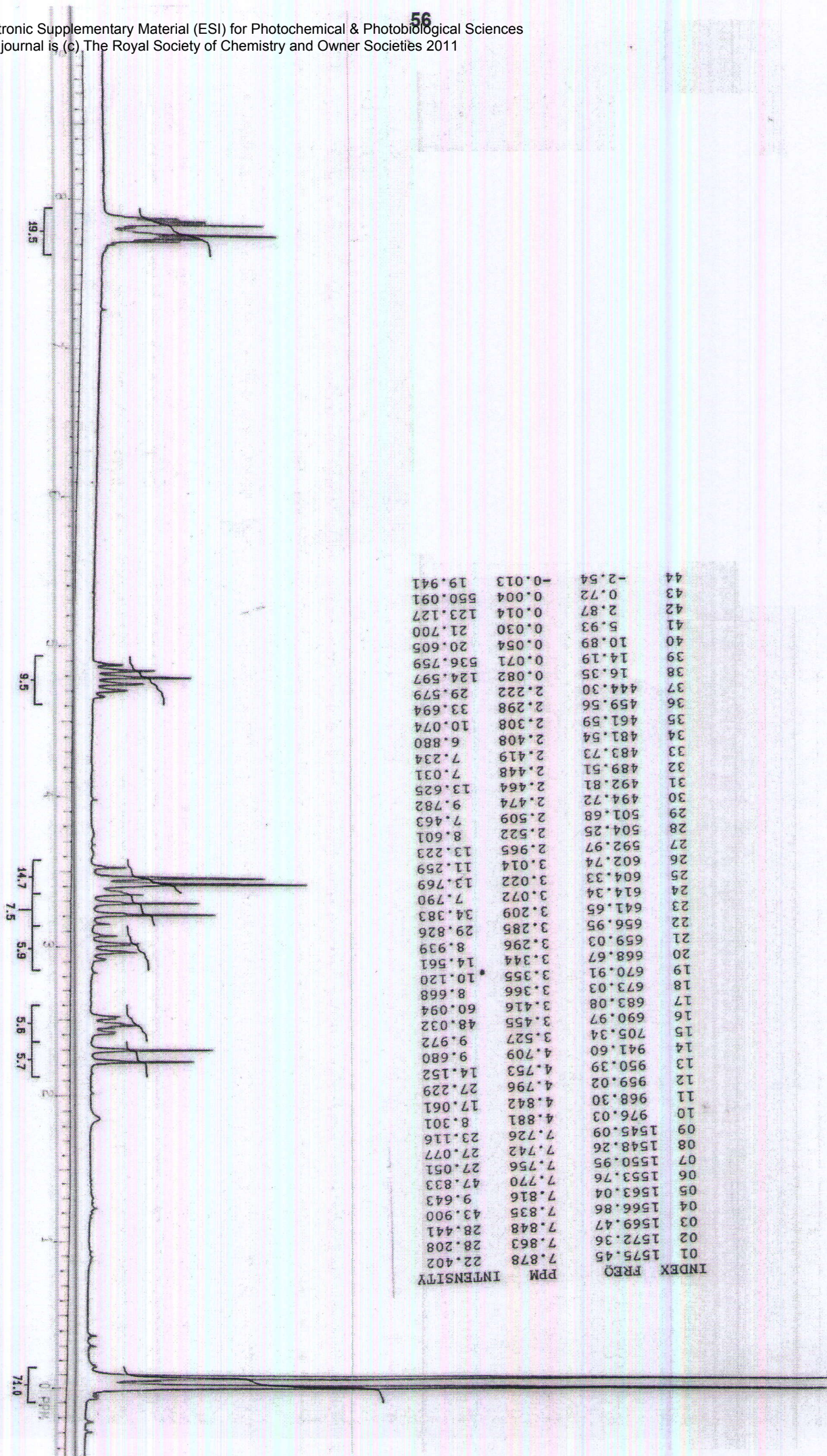


GEMINI-200
 SPECTRAL LINES FOR TH- 7.40
 RFL= 428.7 RPP= 0

INDEX	FREQ	PPM	INTENSITY
01	1580.41	7.903	28.094
02	1577.04	7.886	42.160
03	1575.20	7.877	39.982
04	1571.99	7.861	54.313
05	1568.69	7.844	18.790
06	1558.07	7.791	79.306
07	1555.51	7.778	52.287
08	1553.67	7.769	48.480
09	1550.54	7.754	29.948
10	1450.75	7.255	11.915
11	996.91	4.985	14.027
12	988.49	4.943	30.417
13	979.33	4.897	27.046
14	974.65	4.874	13.578
15	965.78	4.829	23.176
16	956.41	4.783	16.838
17	698.02	3.491	12.168
18	690.24	3.452	20.910
19	688.57	3.443	21.903
20	679.25	3.397	12.238
21	677.87	3.390	11.885
22	660.29	3.302	36.453
23	645.27	3.227	42.470
24	618.90	3.095	10.702
25	608.36	3.042	23.934
26	597.28	2.987	22.791
27	587.23	2.937	9.806
28	518.98	2.595	12.949
29	516.62	2.583	13.934
30	507.26	2.537	22.046
31	504.25	2.522	13.257
32	496.11	2.481	10.721
33	495.09	2.476	9.957
34	454.43	2.272	42.419
35	439.41	2.197	36.967
36	328.06	1.641	48.143
37	6.46	0.032	529.784

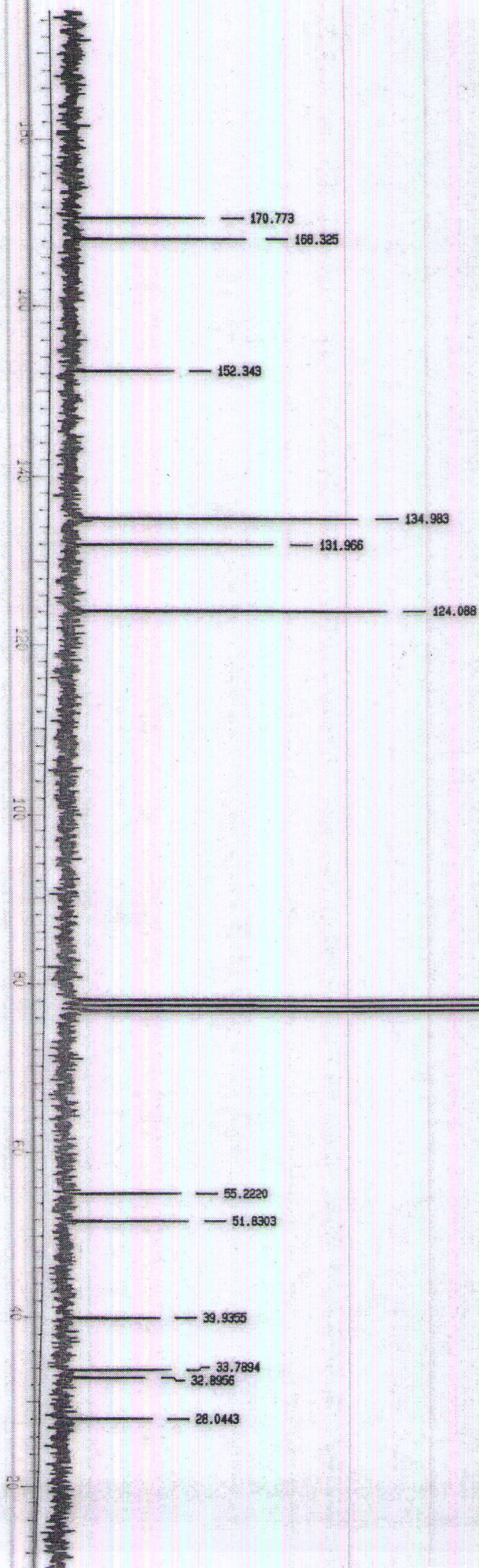
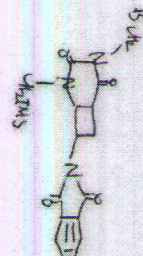
PPM	INTENSITY
171.881	20.005
168.288	49.934
151.552	14.774
135.058	77.613
131.940	54.011
124.176	81.926
124.176	166.573
77.829	173.930
76.894	169.023
56.894	31.676
51.821	33.155
38.541	24.184
33.813	26.207
27.283	24.610
-1.156	100.981

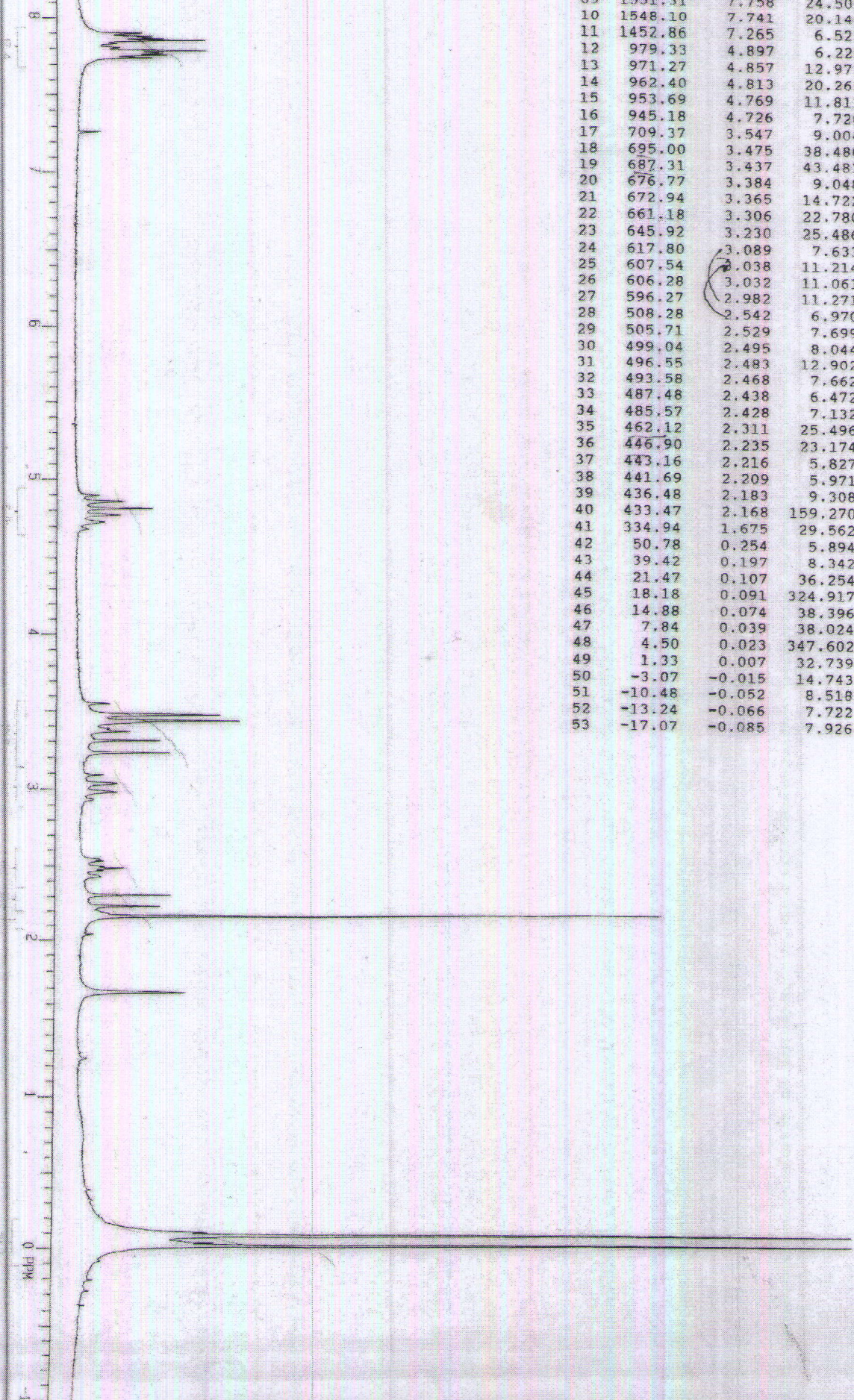




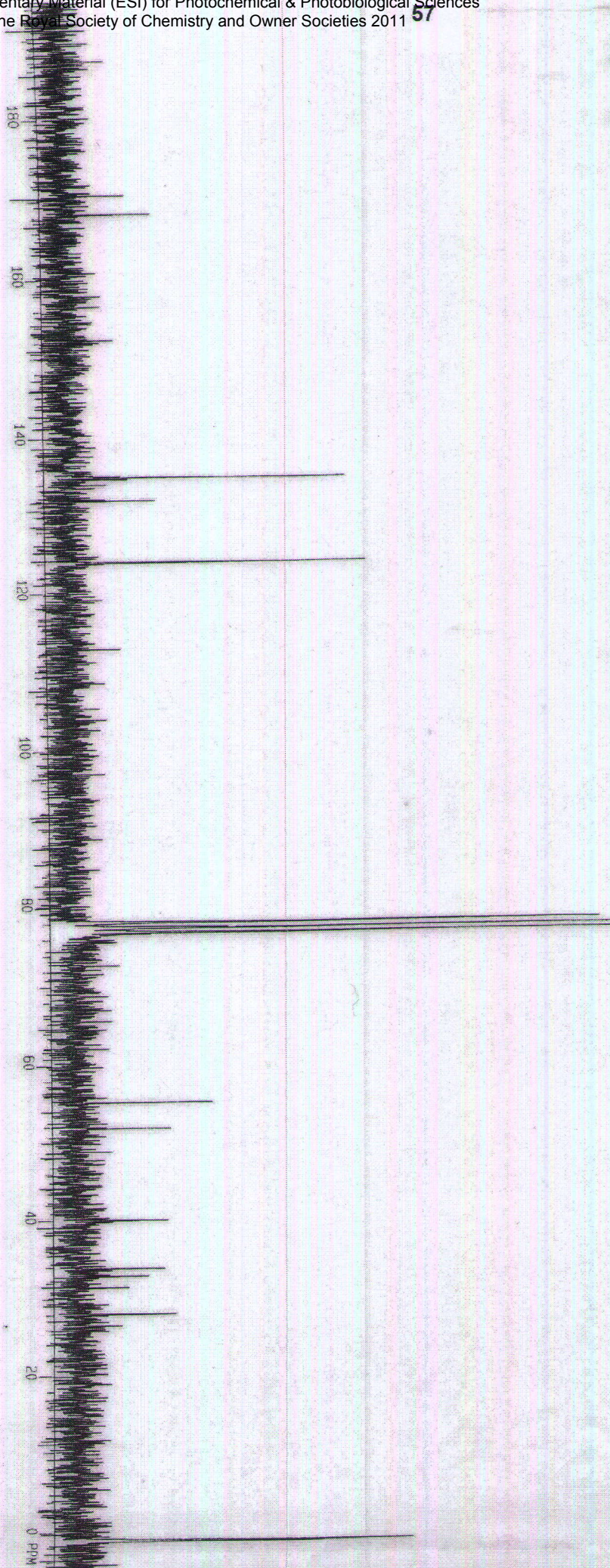
GEMINI-200 13C OBSERVE
 SPECTRAL LINES FOR TH= 15.02
 RFL= 862.8 RFP= 0

INDEX	FREQ	PPM	INTENSITY
01	8588.1	170.773	32.019
02	8465.0	168.325	42.686
03	7661.2	152.343	24.529
04	6788.2	134.983	69.649
05	6636.5	131.965	49.269
06	6240.3	124.088	76.481
07	3931.3	78.173	112.541
08	3899.3	77.537	115.746
09	3867.4	76.902	113.123
10	2777.1	55.222	28.152
11	2606.5	51.830	30.231
12	2008.3	39.936	23.307
13	1699.2	33.789	26.420
14	1654.3	32.896	20.378
15	1410.3	28.044	21.933
16	-54.2	-1.077	103.413
17	-58.8	-1.170	99.338

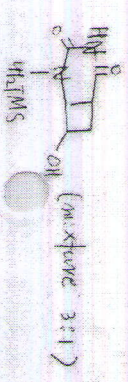
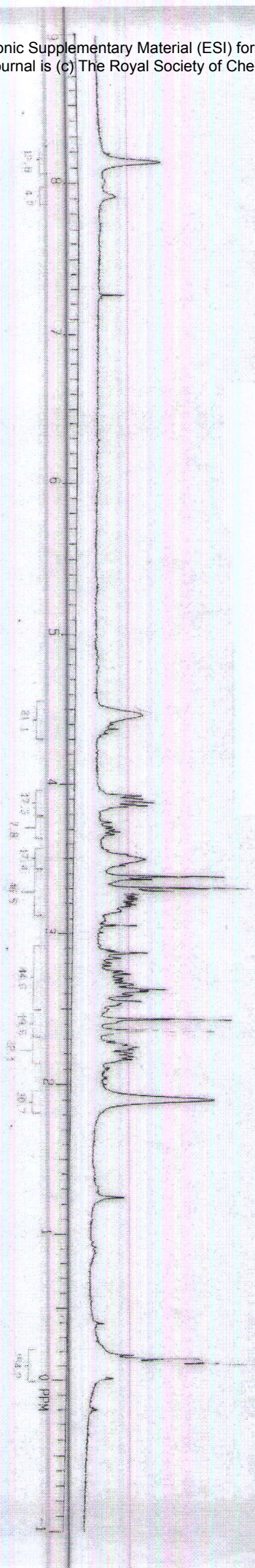




INDEX	FREQ	PPM	INTENSITY
01	1579.23	7.897	17.714
02	1576.02	7.881	20.210
03	1573.45	7.868	23.182
04	1570.52	7.854	34.161
05	1566.13	7.832	10.660
06	1560.63	7.804	11.512
07	1556.69	7.784	34.793
08	1553.31	7.768	22.727
09	1551.31	7.758	24.505
10	1548.10	7.741	20.144
11	1452.86	7.265	6.521
12	979.33	4.897	6.220
13	971.27	4.857	12.973
14	962.40	4.813	20.261
15	953.69	4.769	11.813
16	945.18	4.726	7.720
17	709.37	3.547	9.004
18	695.00	3.475	38.480
19	687.31	3.437	43.483
20	676.77	3.384	9.048
21	672.94	3.365	14.722
22	661.18	3.306	22.780
23	645.92	3.230	25.486
24	617.80	3.089	7.633
25	607.54	3.038	11.214
26	606.28	3.032	11.061
27	596.27	2.982	11.271
28	508.28	2.542	6.970
29	505.71	2.529	7.699
30	499.04	2.495	8.044
31	496.55	2.483	12.902
32	493.58	2.468	7.662
33	487.48	2.438	6.472
34	485.57	2.428	7.132
35	462.12	2.311	25.496
36	446.90	2.235	23.174
37	443.16	2.216	5.827
38	441.69	2.209	5.971
39	436.48	2.183	9.308
40	433.47	2.168	159.270
41	334.94	1.675	29.562
42	50.78	0.254	5.894
43	39.42	0.197	8.342
44	21.47	0.107	36.254
45	18.18	0.091	324.917
46	14.88	0.074	38.396
47	7.84	0.039	38.024
48	4.50	0.023	347.602
49	1.33	0.007	32.739
50	-3.07	-0.015	14.743
51	-10.48	-0.052	8.518
52	-13.24	-0.066	7.722
53	-17.07	-0.085	7.926



INDEX	FREQ	PPM	INTENS
*01	9623.6	191.364	-12.7
02	9415.0	187.216	12.7
03	8590.1	170.814	17.6
*04	8573.1	170.475	-13.3
05	8467.0	168.365	23.8
06	7661.4	152.346	13.4
07	6789.1	135.001	73.1
08	6777.8	134.776	17.8
09	6636.7	131.971	23.7
10	6241.8	124.118	78.0
11	5672.7	112.802	15.3
12	3935.7	78.261	16.0
13	3929.9	78.146	138.2
14	3925.1	78.051	22.1
15	3923.0	78.008	15.2
16	3920.8	77.965	15.4
17	3897.9	77.509	141.9
18	3892.9	77.409	22.0
19	3889.8	77.348	18.3
20	3888.3	77.319	16.6
21	3884.6	77.245	15.6
22	3881.2	77.178	15.4
23	3875.7	77.069	18.7
24	3866.0	76.874	142.2
25	3856.2	76.680	21.0
26	3851.2	76.581	12.5
27	3848.2	76.522	13.2
28	3809.4	75.749	12.2
29	3656.2	72.704	12.8
30	2776.5	55.211	37.2
31	2606.7	51.835	25.6
32	2009.0	39.950	25.0
33	1700.0	33.803	24.0
34	1655.6	32.921	19.9
35	1580.2	31.423	14.5
36	1411.5	28.067	26.8
37	1334.1	26.529	12.5
38	-53.8	-1.069	87.9
39	-58.6	-1.166	83.6
40	-61.8	-1.229	19.5

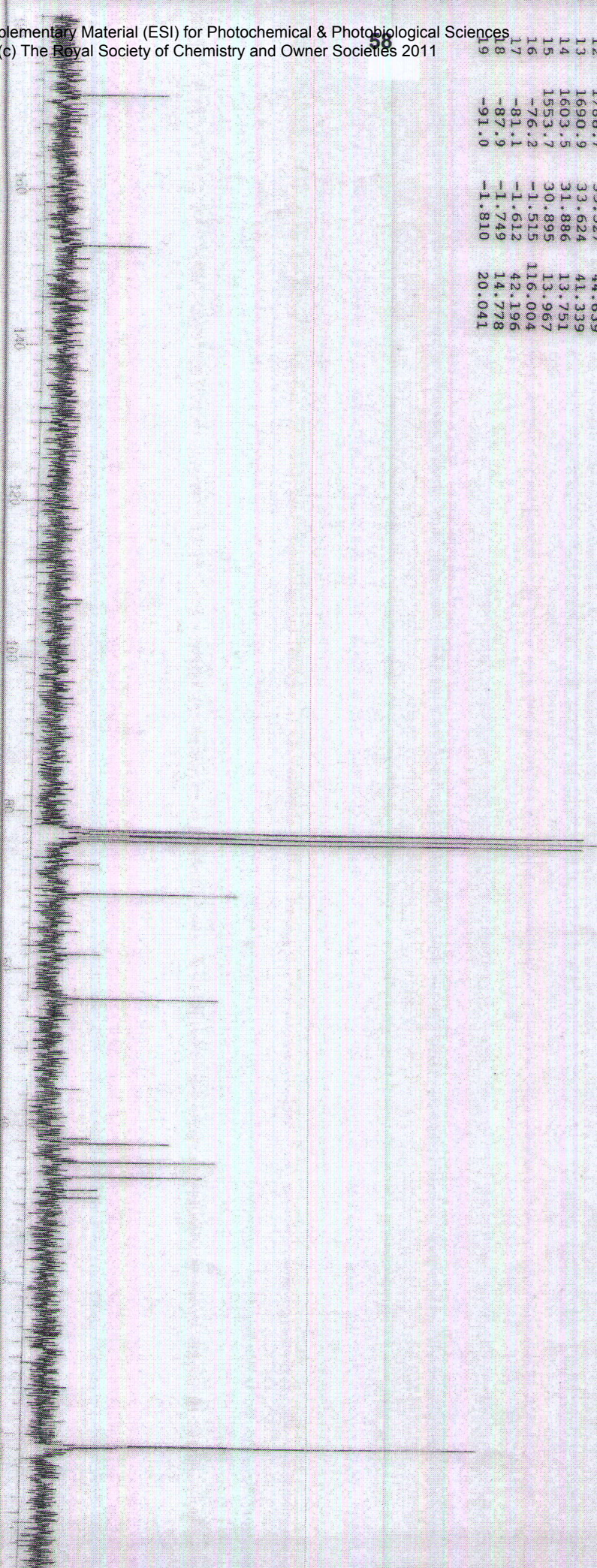


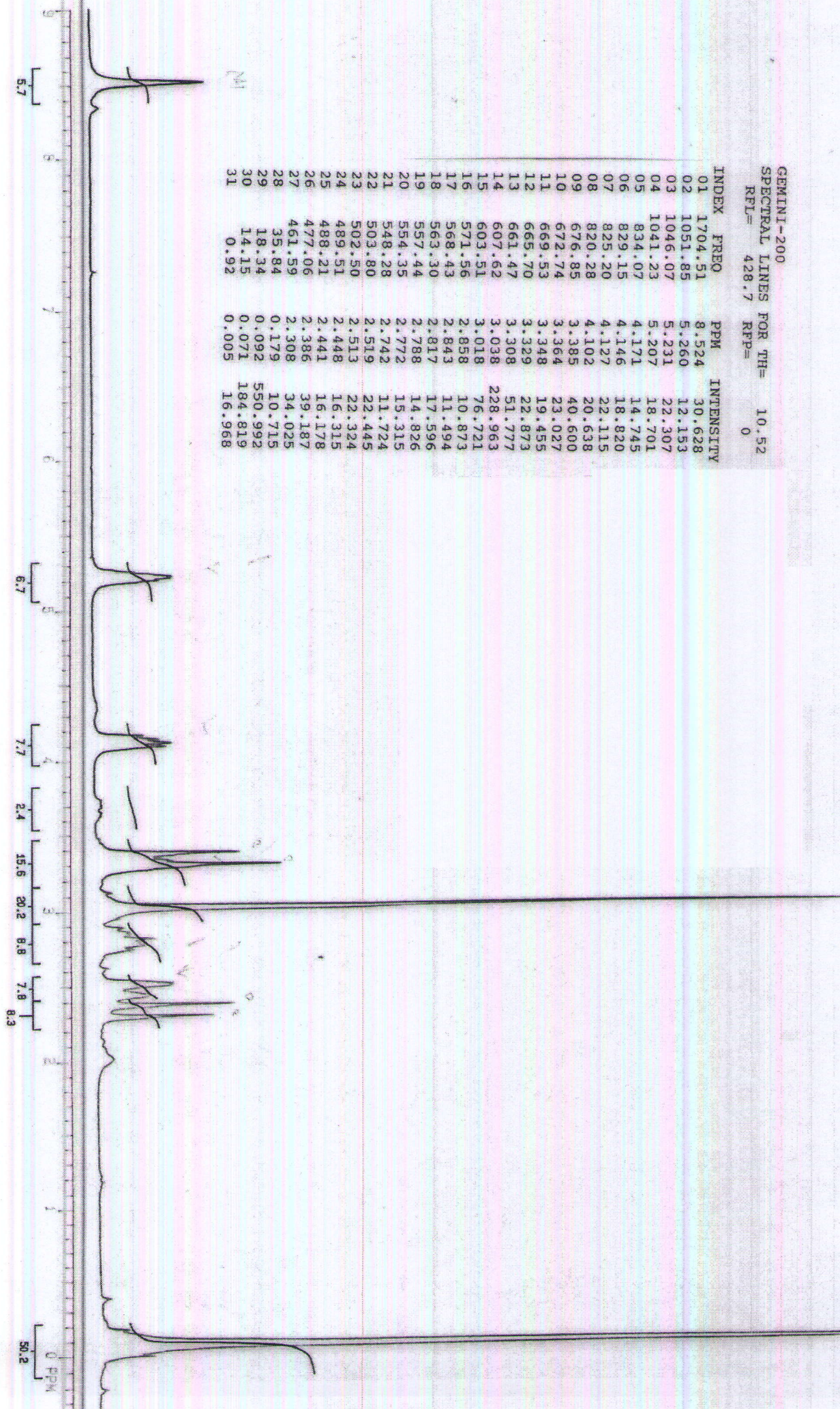
LINES FOR TH= 7.00
 428.7 RFP= 0

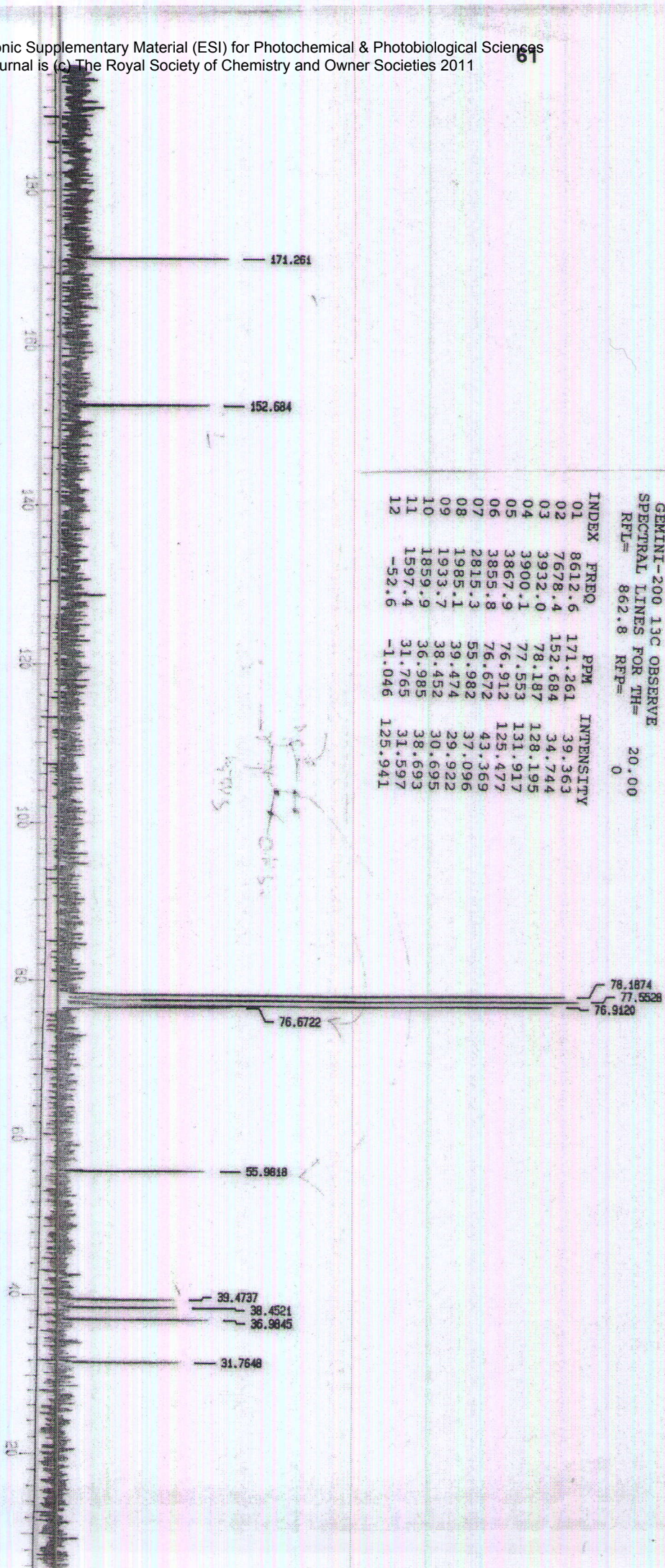
INDEX	FREQ	PPM	INTENSITY
01	1627.58	8.139	13.260
02	893.17	4.466	10.188
03	785.23	3.927	10.099
04	784.09	3.921	7.755
05	780.55	3.903	10.540
06	776.44	3.883	12.619
07	771.72	3.859	11.350
08	705.34	3.527	7.474
09	699.89	3.500	11.118
10	697.28	3.487	9.779
11	694.64	3.474	7.711
12	676.77	3.384	27.243
13	672.54	3.363	12.790
14	661.43	3.308	32.953
15	657.15	3.286	17.520
16	654.59	3.273	8.792
17	652.07	3.261	9.789
18	649.75	3.249	8.839
19	647.63	3.239	9.644
20	645.55	3.228	9.441
21	643.07	3.216	8.484
22	640.87	3.205	8.136
23	638.64	3.194	9.036
24	636.40	3.182	8.023
25	611.57	3.058	9.290
26	574.66	2.874	11.888
27	546.37	2.732	8.274
28	532.65	2.664	8.956
29	530.66	2.654	7.042
30	526.27	2.632	15.621
31	524.23	2.621	11.906
32	518.53	2.593	8.566
33	510.84	2.555	10.509
34	487.44	2.437	29.313
35	472.05	2.361	25.594
36	453.25	2.267	7.969
37	450.24	2.251	10.432
38	448.86	2.245	8.798
39	446.90	2.235	9.157
40	445.97	2.230	8.352
41	441.24	2.206	8.655
42	440.15	2.201	7.286
43	437.17	2.186	8.975
44	432.82	2.164	8.656
45	381.99	1.910	25.911
46	249.59	1.248	7.396
47	35.56	0.178	10.168
48	31.16	0.156	25.018
49	25.87	0.129	27.847
50	22.57	0.113	202.426
51	20.21	0.101	441.940
52	12.68	0.063	16.381

GEMINI-200
SPECTRAL LINES FOR TH= 11.11
RFL= 4760.5 RPD= 3872.3

INDEX	FREQ	PPM	INTENSITY
01	8649.9	172.003	27.856
02	7679.7	152.711	22.459
03	3904.2	77.635	139.143
04	3872.3	77.000	143.416
05	3840.4	76.365	138.823
06	3692.4	73.422	12.720
07	3508.1	69.757	49.190
08	3119.2	62.025	13.452
09	2829.9	56.272	44.574
10	1932.2	38.421	11.681
11	1901.6	37.814	32.369
12	1786.7	35.527	44.639
13	1690.9	33.624	41.339
14	1603.5	31.886	13.751
15	1553.7	30.895	13.967
16	-76.2	-1.515	116.004
17	-81.1	-1.612	42.196
18	-87.9	-1.749	14.778
19	-91.0	-1.810	20.041

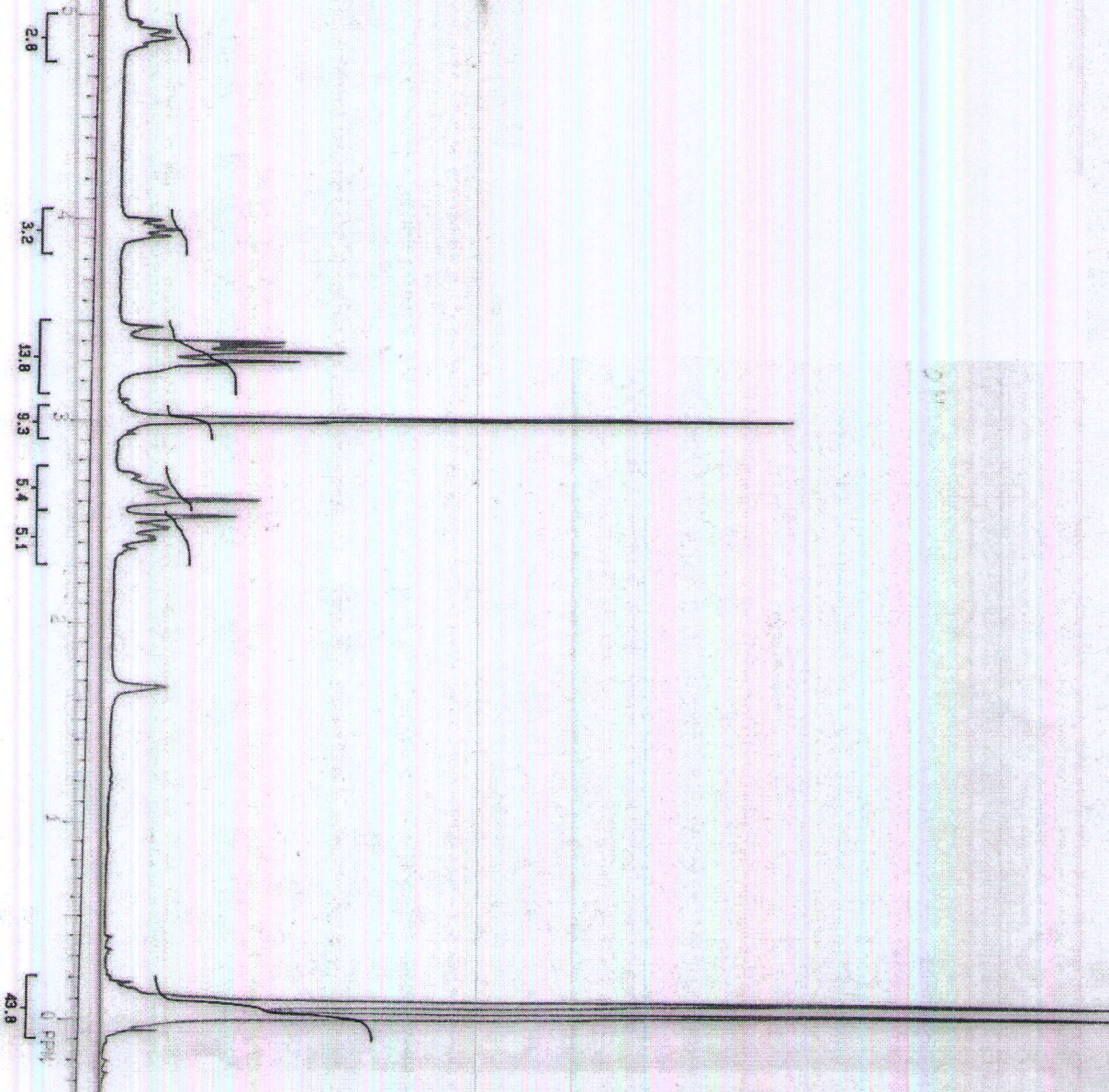






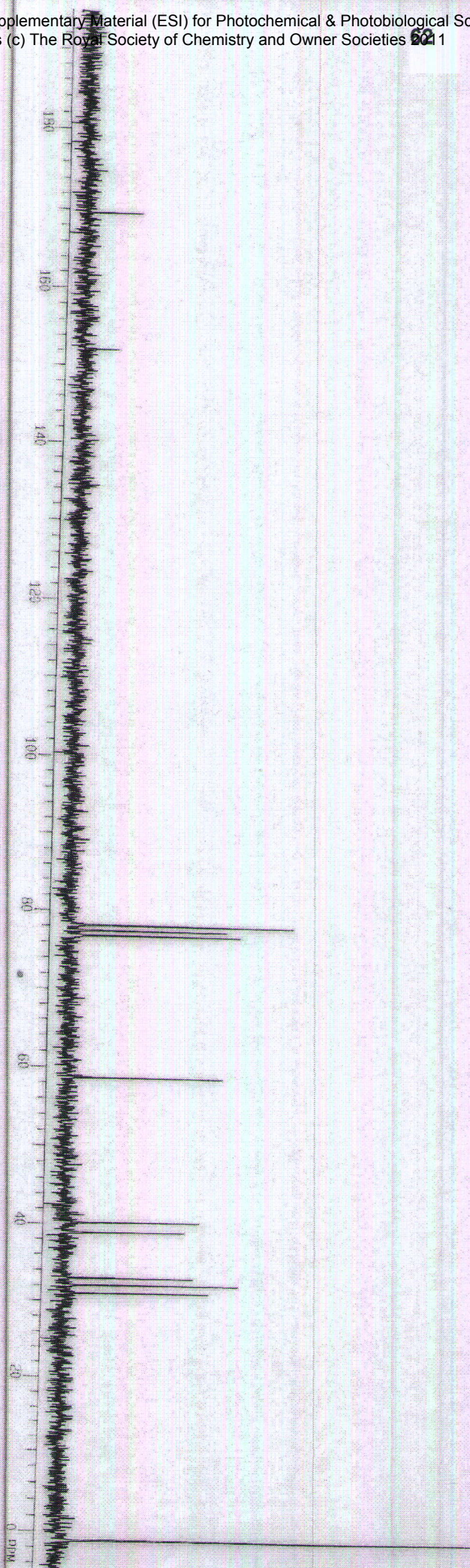
GEMINI-200
 SPECTRAL LINES FOR TH= 4.92
 RFL= 428.7 RFP= 0

INDEX	FREQ	PPM	INTENSITY
01	984.82	4.925	9.294
02	978.31	4.892	10.232
03	799.48	3.998	8.419
04	793.17	3.966	9.088
05	789.22	3.947	12.300
06	782.91	3.915	10.152
07	695.09	3.476	8.949
08	680.43	3.403	33.470
09	676.57	3.383	33.662
10	670.91	3.355	45.574
11	661.18	3.306	37.041
12	656.62	3.284	21.608
13	652.15	3.261	9.979
14	604.20	3.021	135.215
15	599.89	3.000	42.664
16	544.62	2.723	5.116
17	532.90	2.665	10.727
18	526.75	2.634	8.977
19	521.83	2.609	29.126
20	506.40	2.532	24.522
21	497.29	2.487	9.135
22	495.09	2.476	11.298
23	493.18	2.466	10.831
24	486.71	2.434	8.290
25	484.63	2.423	8.291
26	482.55	2.413	8.419
27	334.29	1.672	11.074
28	35.84	0.179	5.659
29	24.32	0.122	14.789
30	18.91	0.095	312.654
31	14.51	0.073	104.154
32	7.27	0.036	320.947
33	3.00	0.015	98.273
34	-10.03	-0.050	10.716



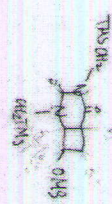
GEMINI-200
SPECTRAL LINES FOR TH= 8.28
RFL= 862.8 RFP= 0

INDEX	FREQ	PPM	INTENSITY
01	8533.1	169.681	14.834
02	7653.7	152.192	9.222
03	3932.1	78.189	59.027
04	3930.1	78.150	47.786
05	3897.9	77.510	41.922
06	3865.8	76.871	45.206
07	2953.4	58.728	41.231
08	2023.5	40.237	35.884
09	1959.3	38.960	32.035
10	1661.2	33.033	34.719
11	1614.3	32.100	46.493
12	1562.2	31.065	39.027
13	-53.3	-1.059	108.581
14	-56.2	-1.117	109.056

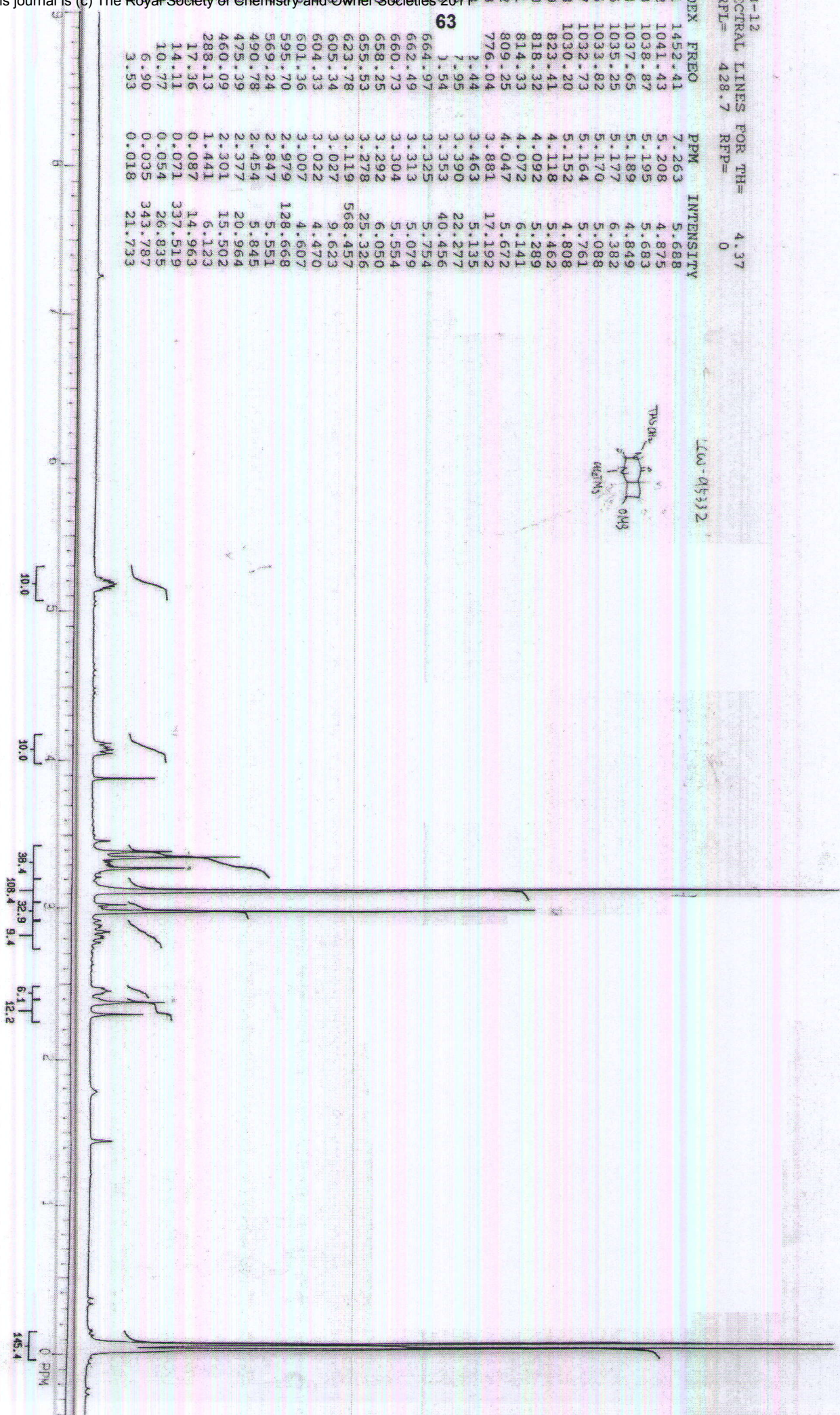


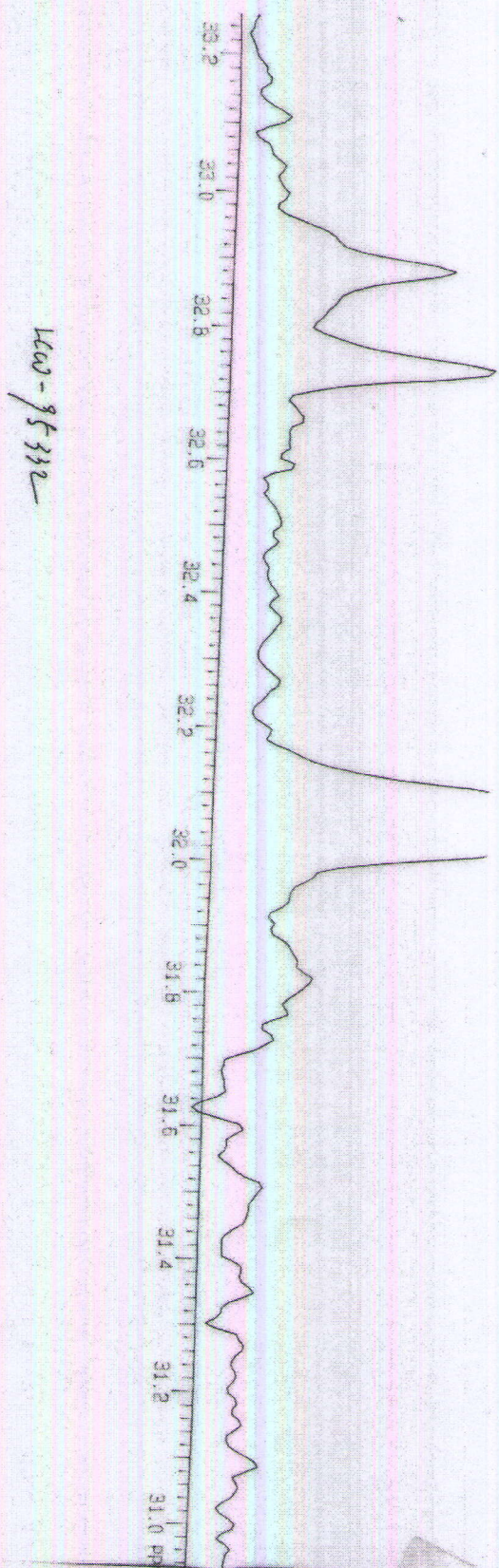
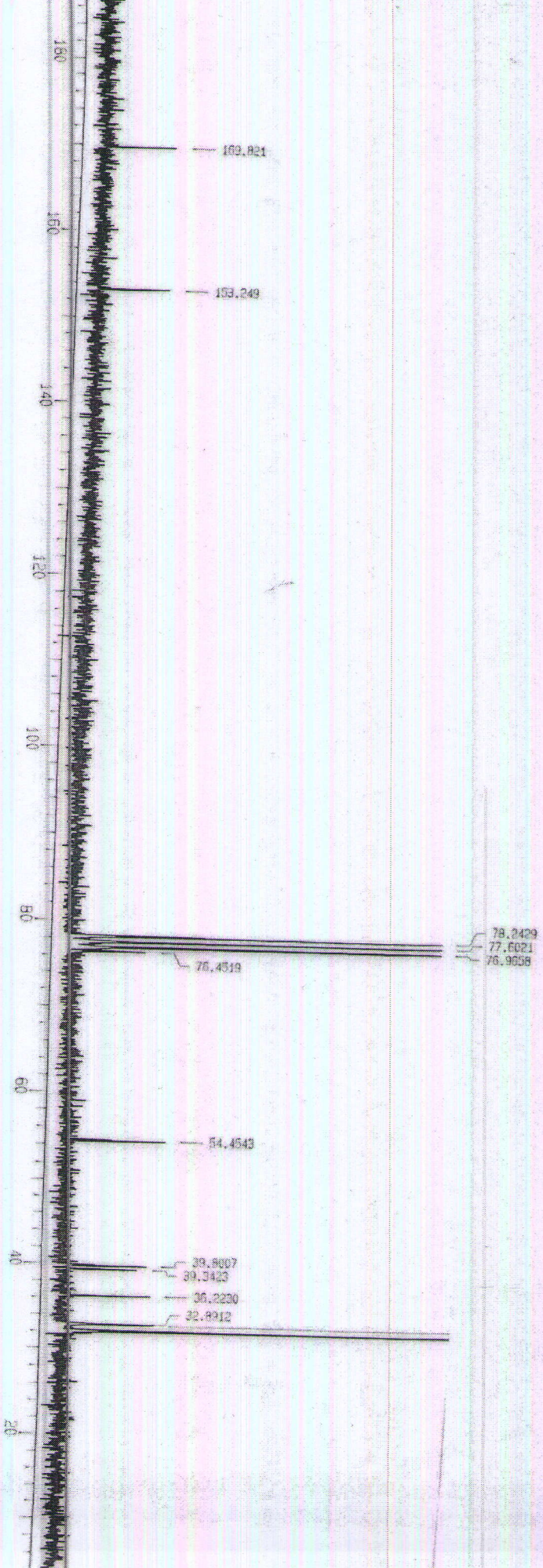
B-3-12
 SPECTRAL LINES FOR TH= 4.37
 RFL= 428.7 RFD= 0

INDEX	FREQ	PPM	INTENSITY
01	1452.41	7.263	5.688
02	1041.43	5.208	4.875
03	1038.87	5.195	5.683
04	1037.65	5.189	4.849
05	1035.25	5.177	6.382
06	1033.82	5.170	5.088
07	1032.73	5.164	5.761
08	1030.20	5.152	4.808
09	823.41	4.118	5.462
10	818.32	4.092	5.289
11	814.33	4.072	6.141
12	809.25	4.047	5.672
13	776.04	3.881	17.192
14	744	3.463	5.135
15	7.95	3.390	22.277
16	1.54	3.353	40.456
17	664.97	3.325	5.754
18	662.49	3.313	5.079
19	660.73	3.304	5.554
20	658.25	3.292	6.050
21	655.53	3.278	25.326
22	623.78	3.119	568.457
23	605.34	3.027	9.623
24	604.33	3.022	4.470
25	601.36	3.007	4.607
26	595.70	2.979	128.668
27	569.24	2.847	5.551
28	490.78	2.454	5.845
29	475.39	2.377	20.964
30	460.09	2.301	15.502
31	288.13	1.441	6.123
32	17.36	0.087	14.963
33	14.11	0.071	337.519
34	10.77	0.054	26.835
35	6.90	0.035	343.787
36	3.53	0.018	21.733



LC03-05332





K-2
 SPECTRAL LINES FOR T1
 RFL= 862.8 RFP=

INDEX	FREQ	PPM
01	8540.2	169.821
02	7706.8	153.249
03	3934.8	78.243
04	3902.6	77.602
05	3870.6	76.966
06	3844.9	76.456
07	2738.4	54.453
08	2001.6	39.802
09	1978.5	39.342
10	1821.7	36.224
11	1654.1	32.891
12	1646.8	32.747
13	1613.0	32.074
14	-48.8	-0.971