Supporting information

Baeyer-Villiger Oxidation in Supercritical CO_2 with Potassium Peroxomonosulfate Supported on Acidic Silica-gel

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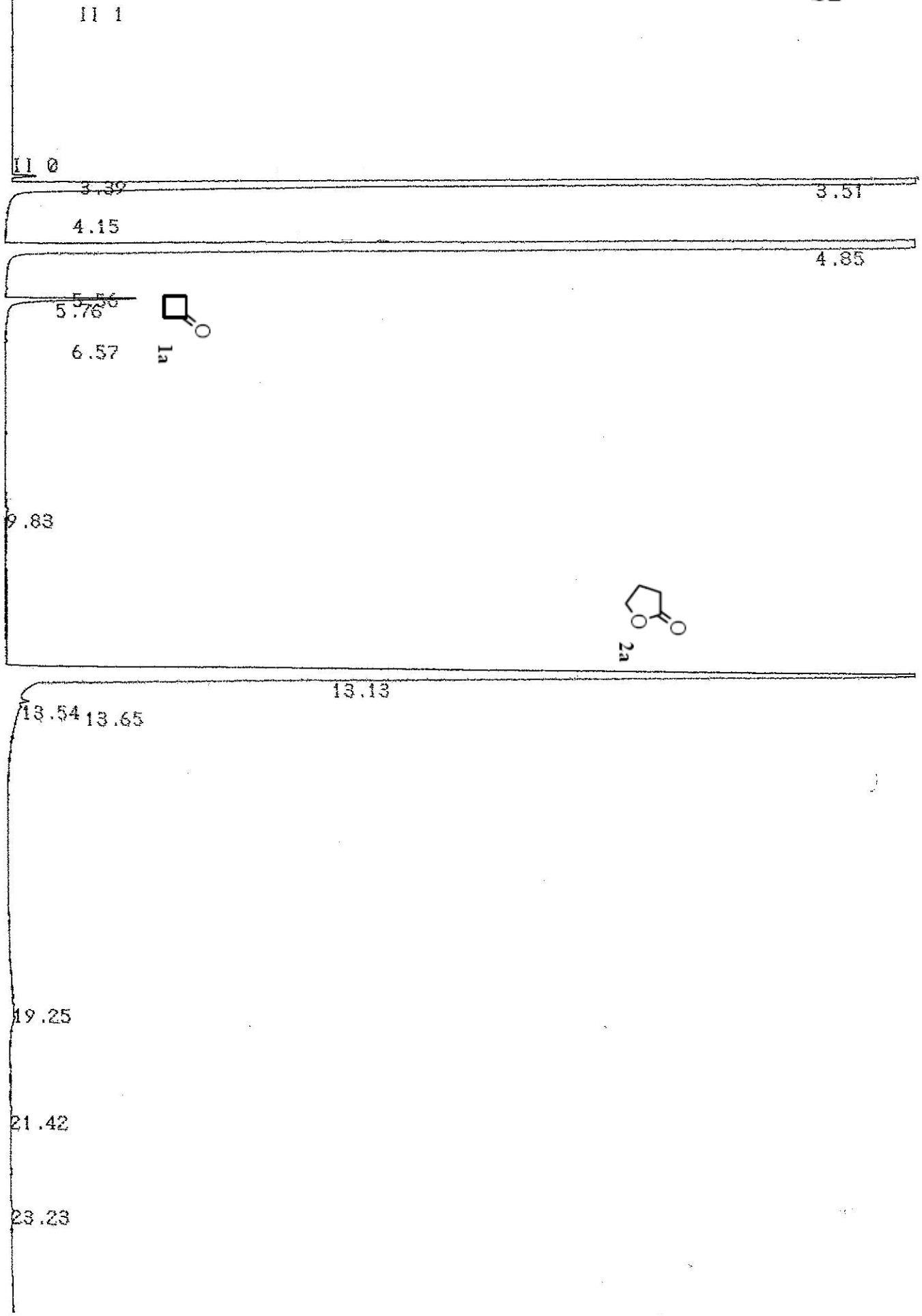
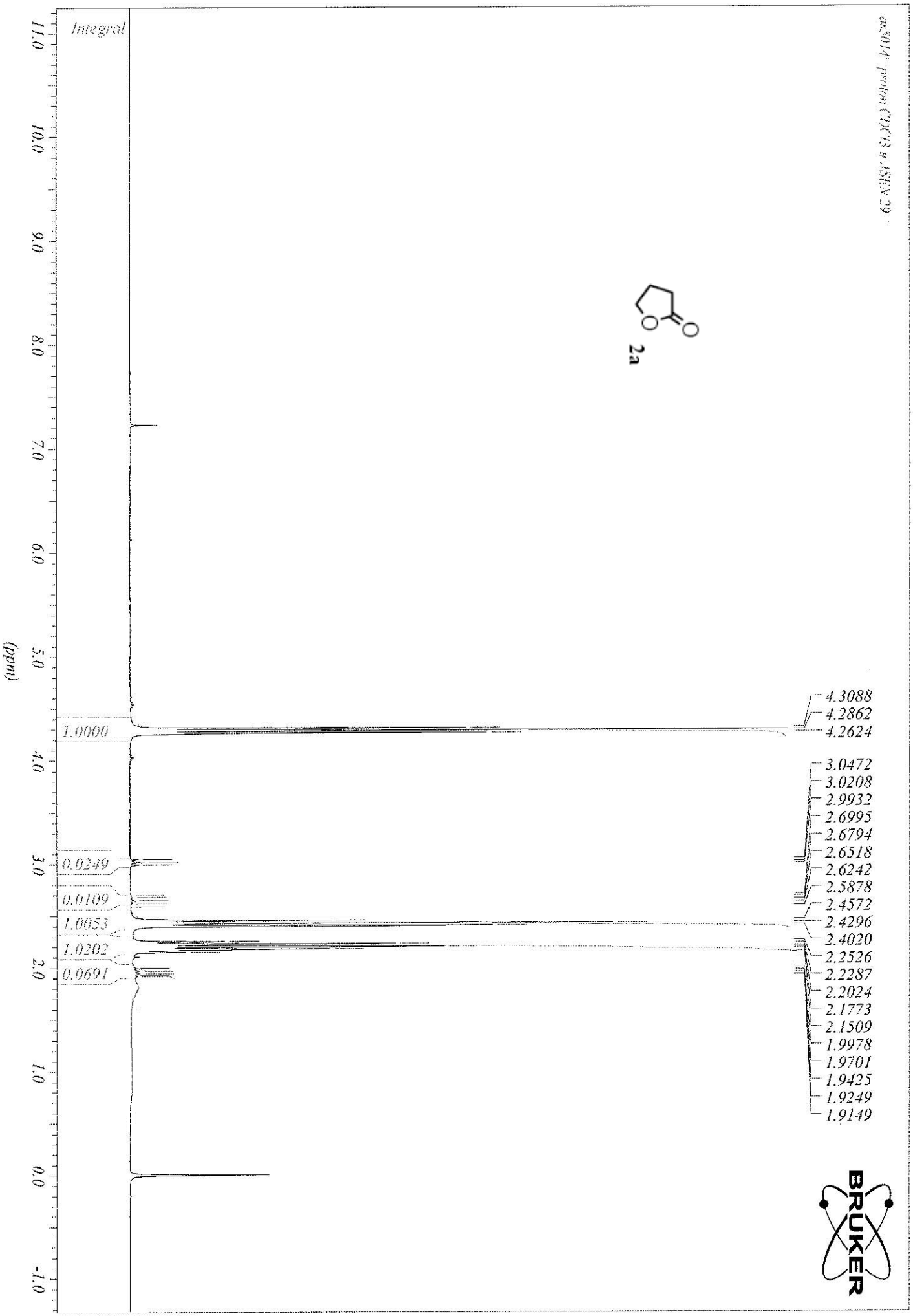
Departamento de Química Orgánica, Universidad de Valencia, Avda. V. Andrés Estellés s/n, 46100-Burjassot (Valencia), Spain

S2-S30: Gas chromatograms, ^{1}H and ^{13}C-NMR spectra of the reaction crudes.

CHANNEL A INJECT 08-06-00 50:22:09 STORED TO BIN # 34

S2

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7.0
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5.0
4.0
3.0
2.0
1.0
0.0
-1.0
1.0000
0.0249
0.0109
1.0053
1.0202
0.0691
4.3088
4.2862
4.2624
3.0472
3.0208
2.9932
2.6995
2.6794
2.6518
2.6242
2.5878
2.4572
2.4296
2.4020
2.2526
2.2287
2.2024
2.1773
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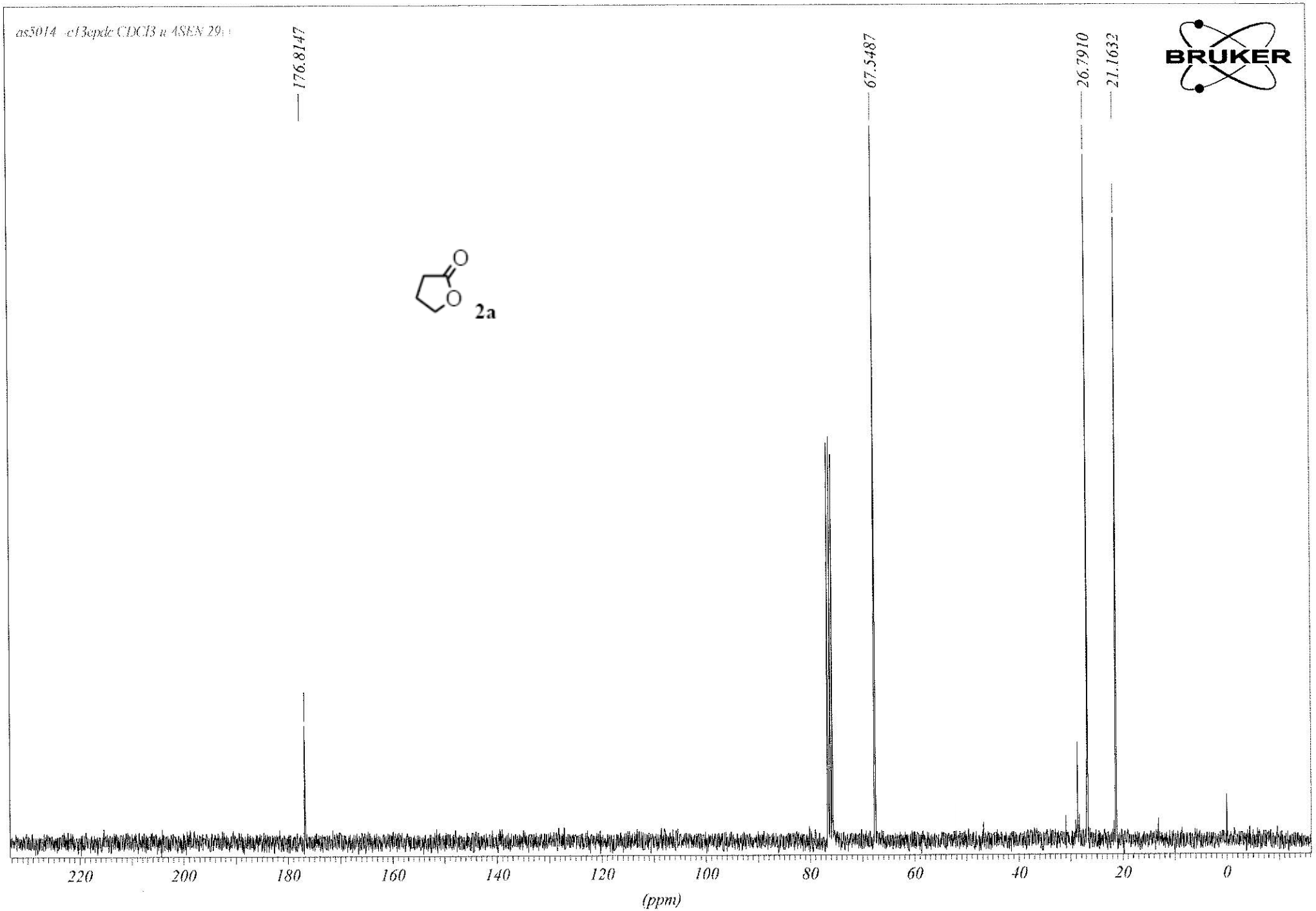
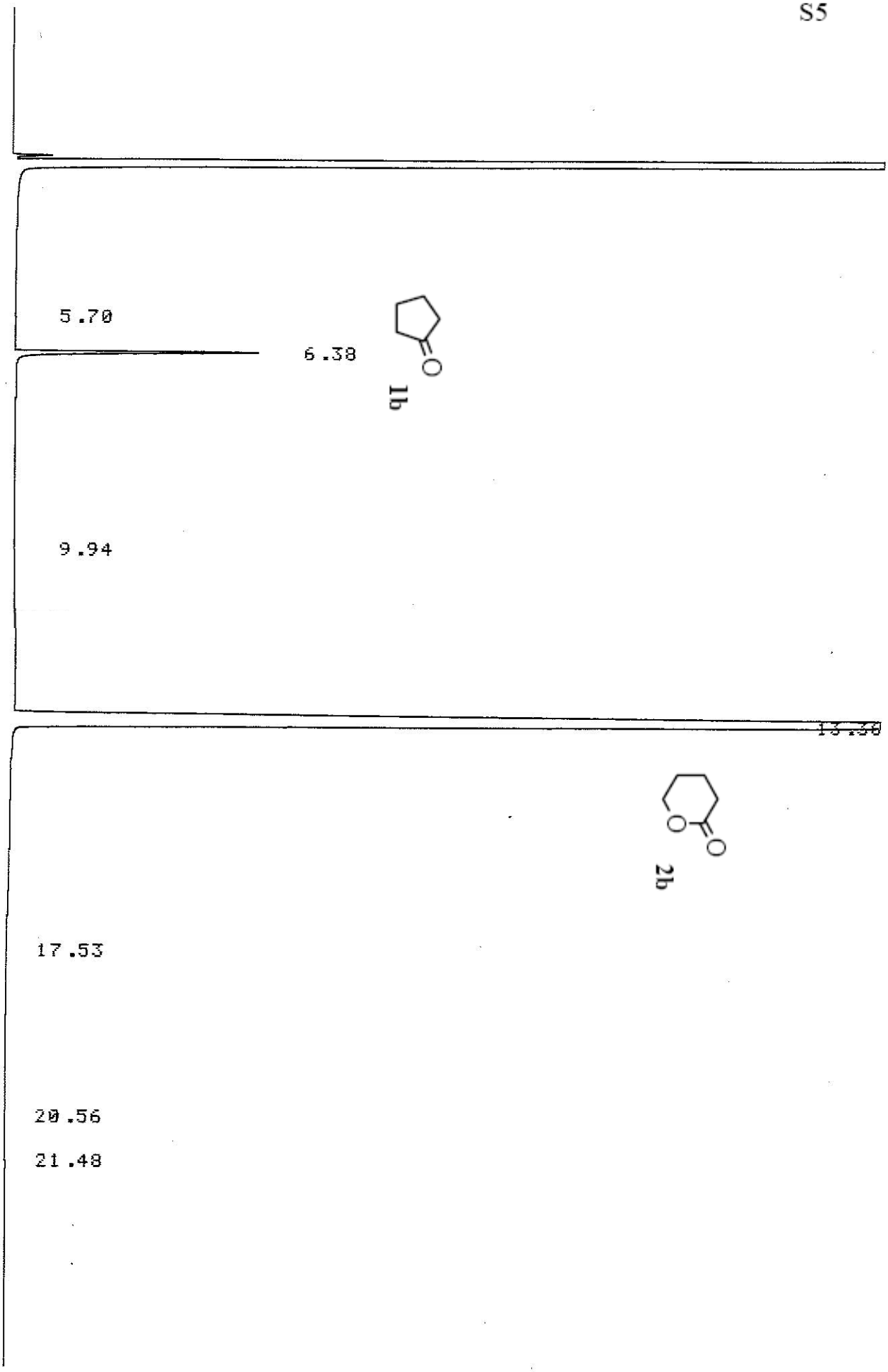
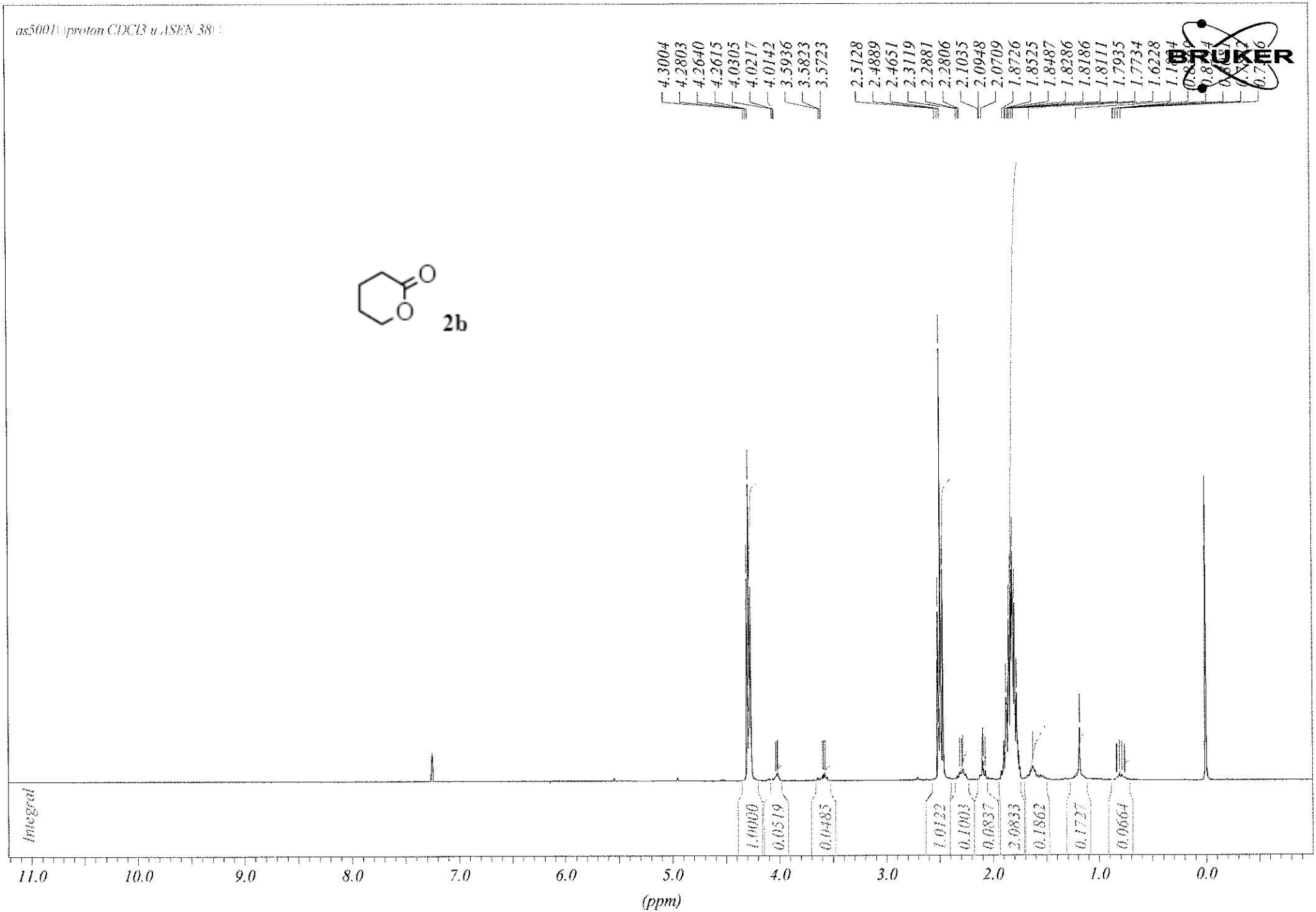
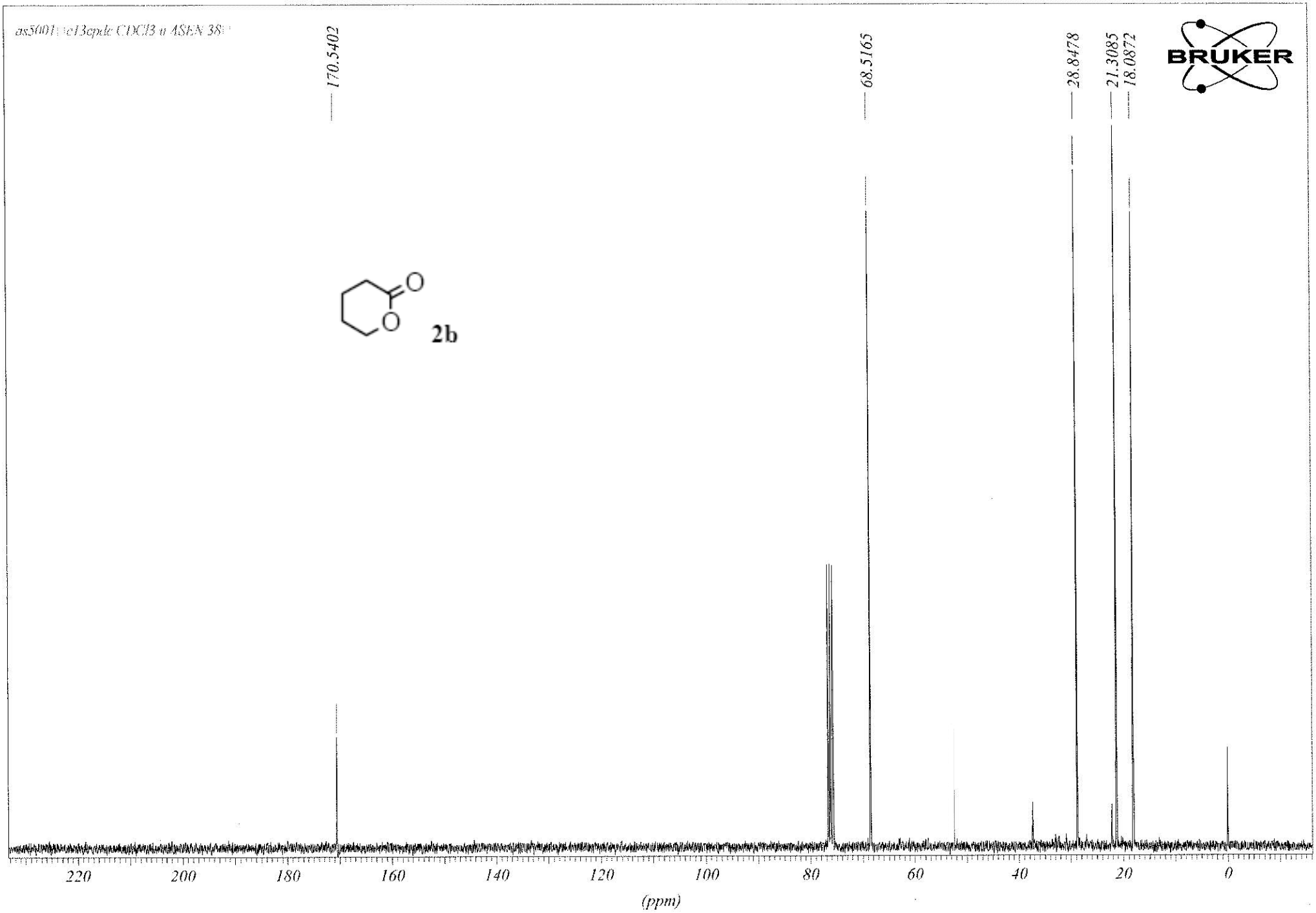
1.9978
1.9701
1.9425
1.9249
1.9149
BRUKER


as5014 -c13epdc CDCl3 u ASEN 29
176.8147
67.5487
26.7910
21.1632
BRUKER
2a
220
200
180
160
140
120
100
80
60
40
20
0
(ppm)

CH. 1 C.5 10.00 ATT 3 OFFS 0 01/11/06 15:39




as5001 | proton CDCl3 u ASEN 38
2b
4.3004
4.2803
4.2640
4.2615
4.0305
4.0217
4.0142
3.5936
3.5823
3.5723
2.5128
2.4889
2.4651
2.3119
2.2881
2.2806
2.1035
2.0948
2.0709
1.8726
1.8525
1.8487
1.8286
1.8186
1.8111
1.7935
1.7734
1.6228
Integral
1.0000
0.0519
0.0485
1.0122
0.1003
0.0837
2.0833
0.1862
0.1727
0.0664
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)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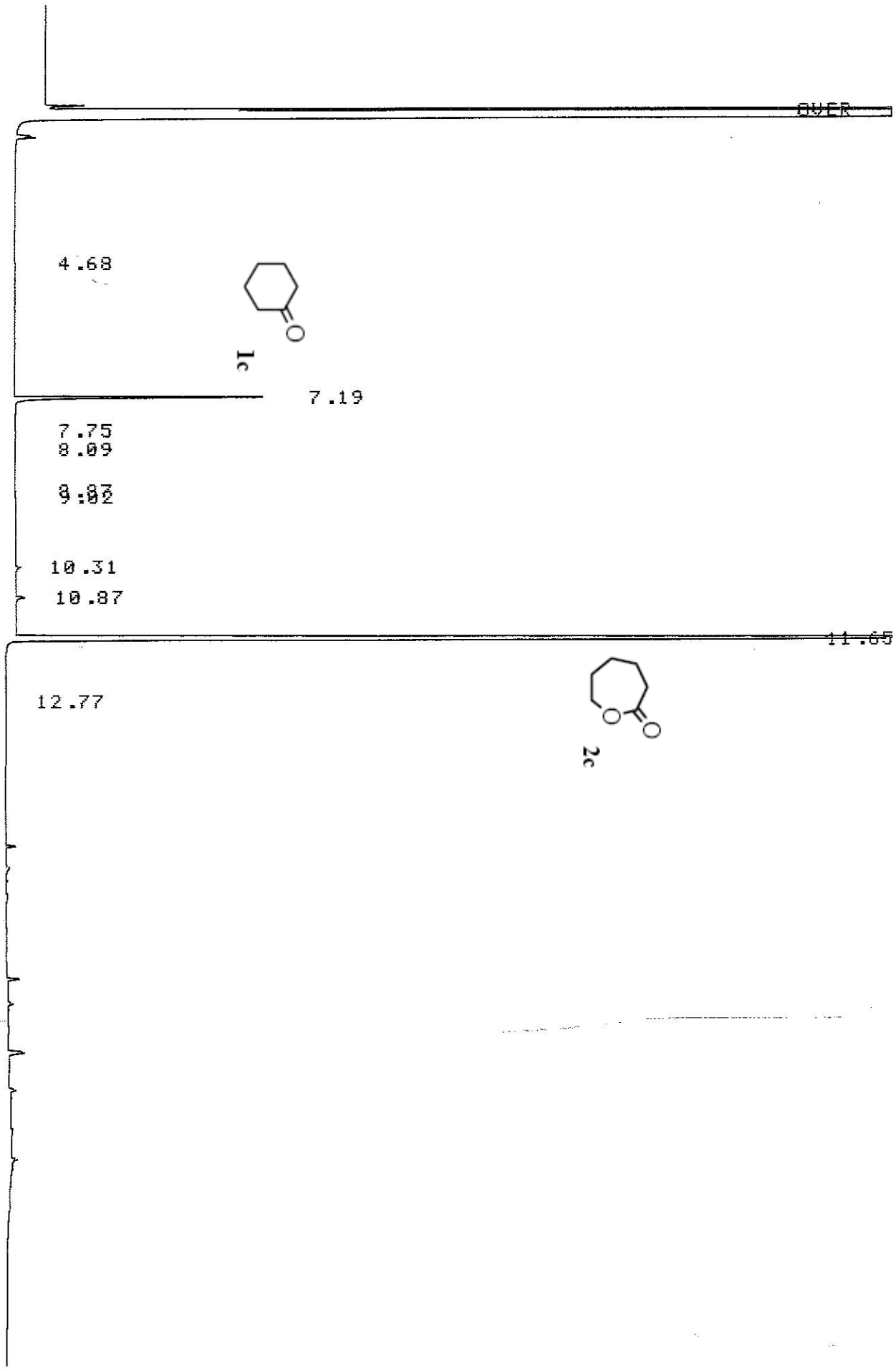
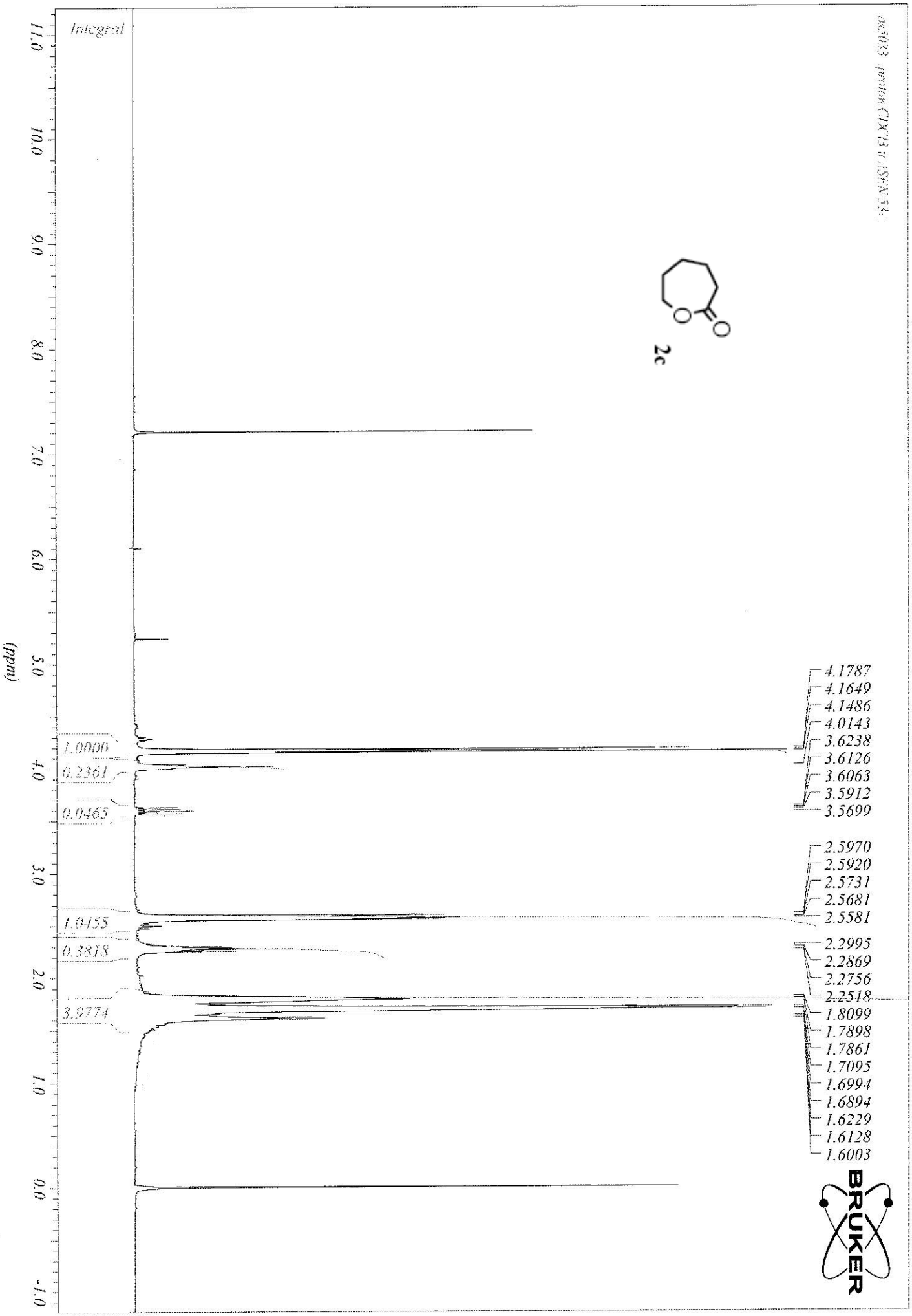
170.5402
68.5165
28.8478
21.3085
18.0872
BRUKER
2b
220
200
180
160
140
120
100
80
60
40
20
0
(ppm)

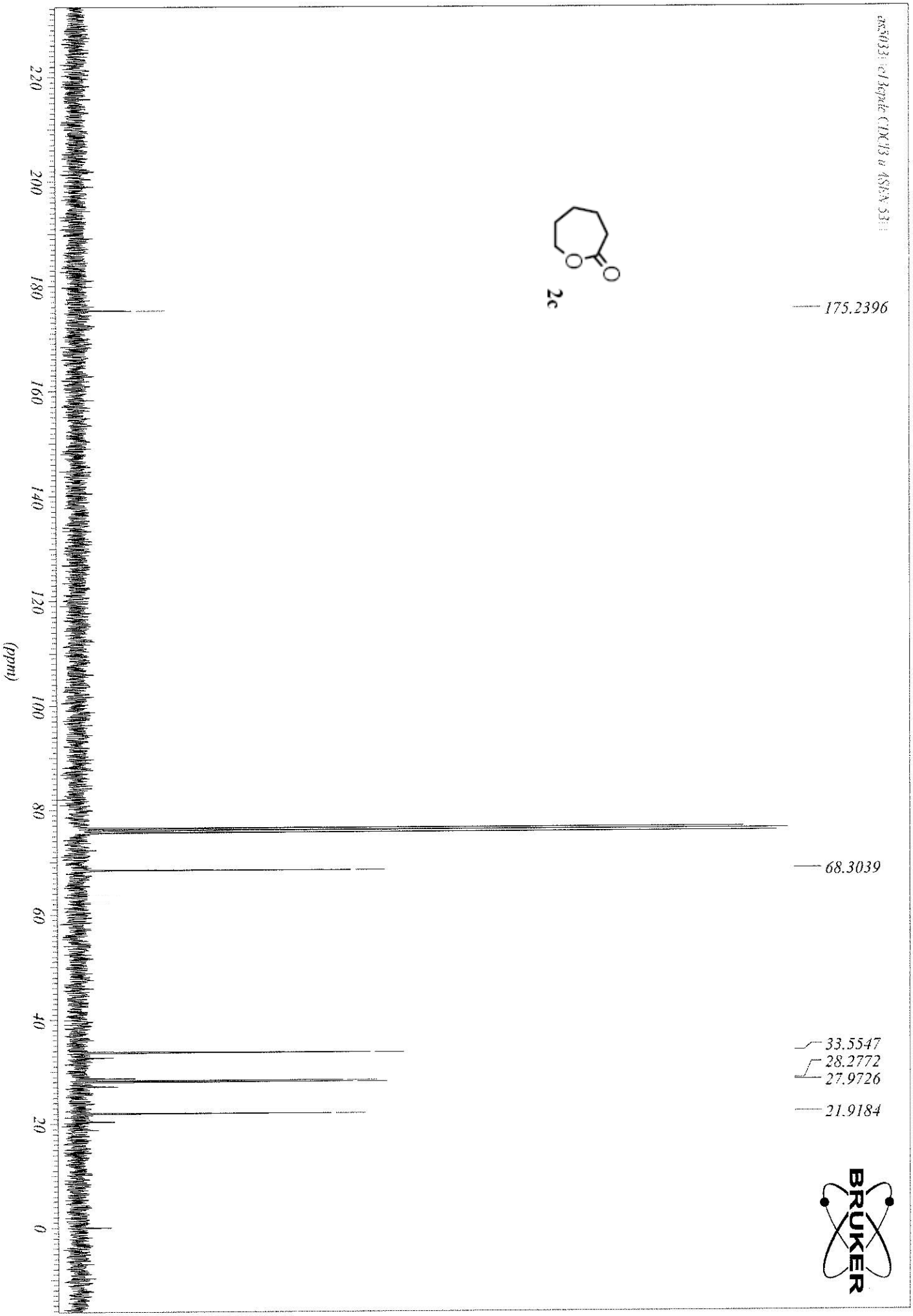
N-AOJ-33 91%

CH. 1 C.S 10.00 ATT 3 OFFS 0 10/13/05 10:39

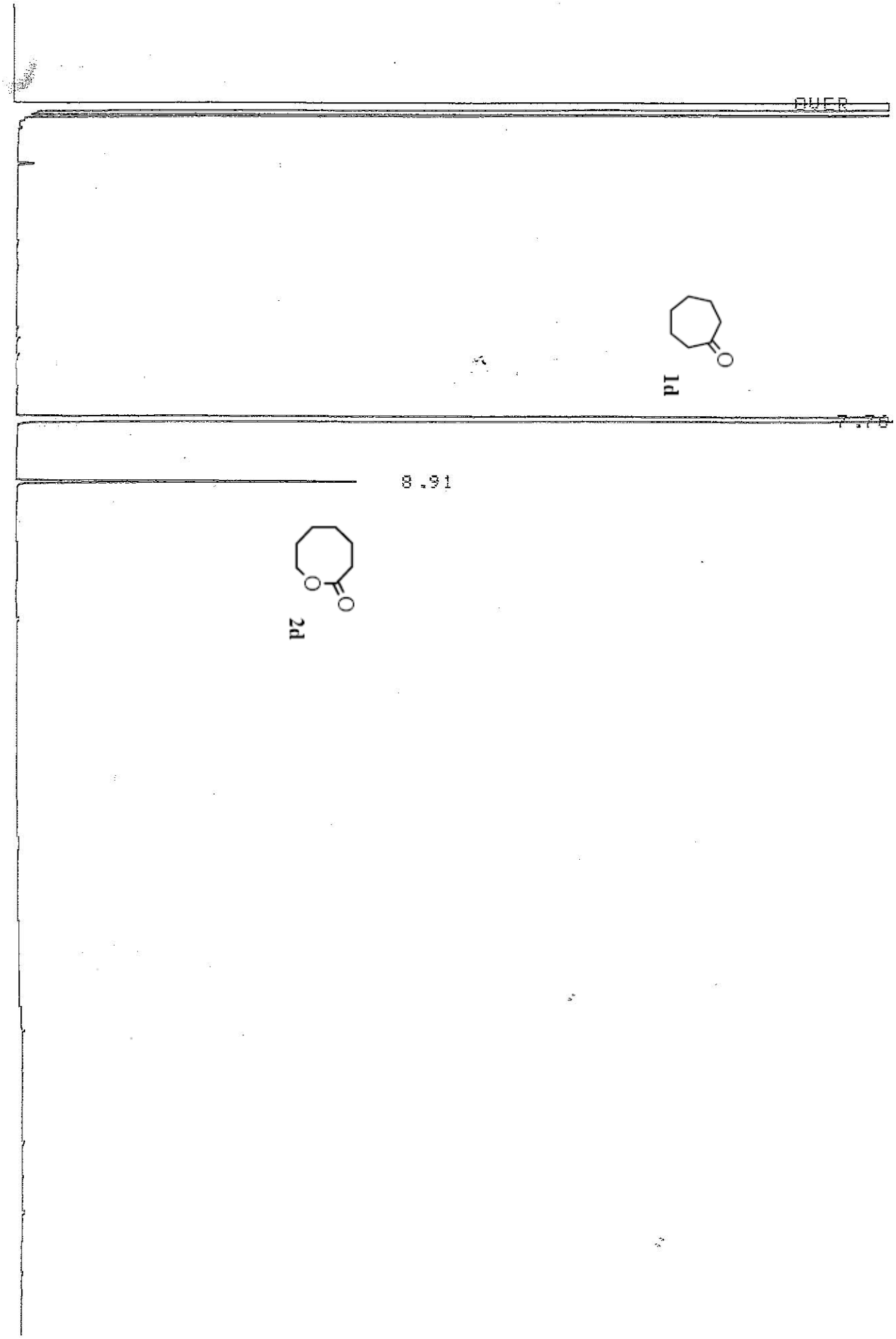


D-2500 10/13/05 10:39

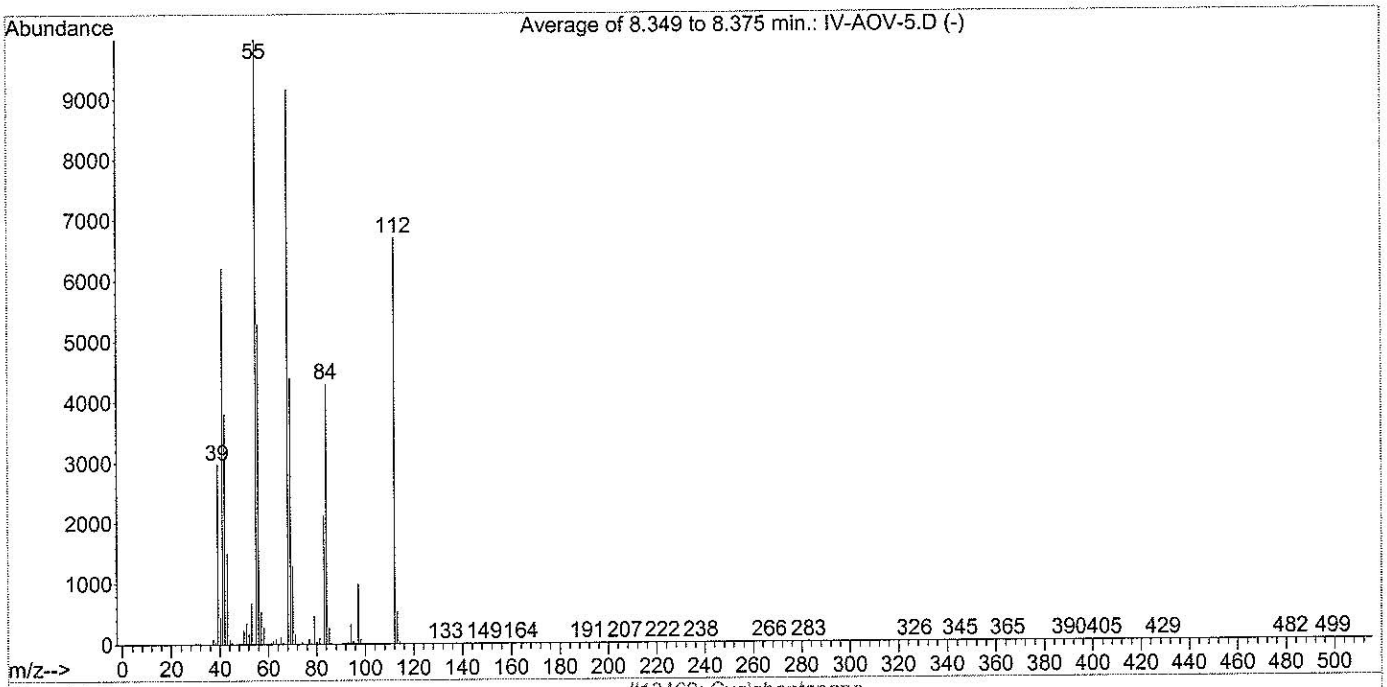

ak3033 proton CDCl3 u ASFN 53
2c
Integral
1.0000
0.2361
0.0465
1.0455
0.3818
3.9774
4.1787
4.1649
4.1486
4.0143
3.6238
3.6126
3.6063
3.5912
3.5699
2.5970
2.5920
2.5731
2.5681
2.5581
2.2995
2.2869
2.2756
2.2518
1.8099
1.7898
1.7861
1.7095
1.6994
1.6894
1.6229
1.6128
1.6003
(ppm)
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
BRUKER

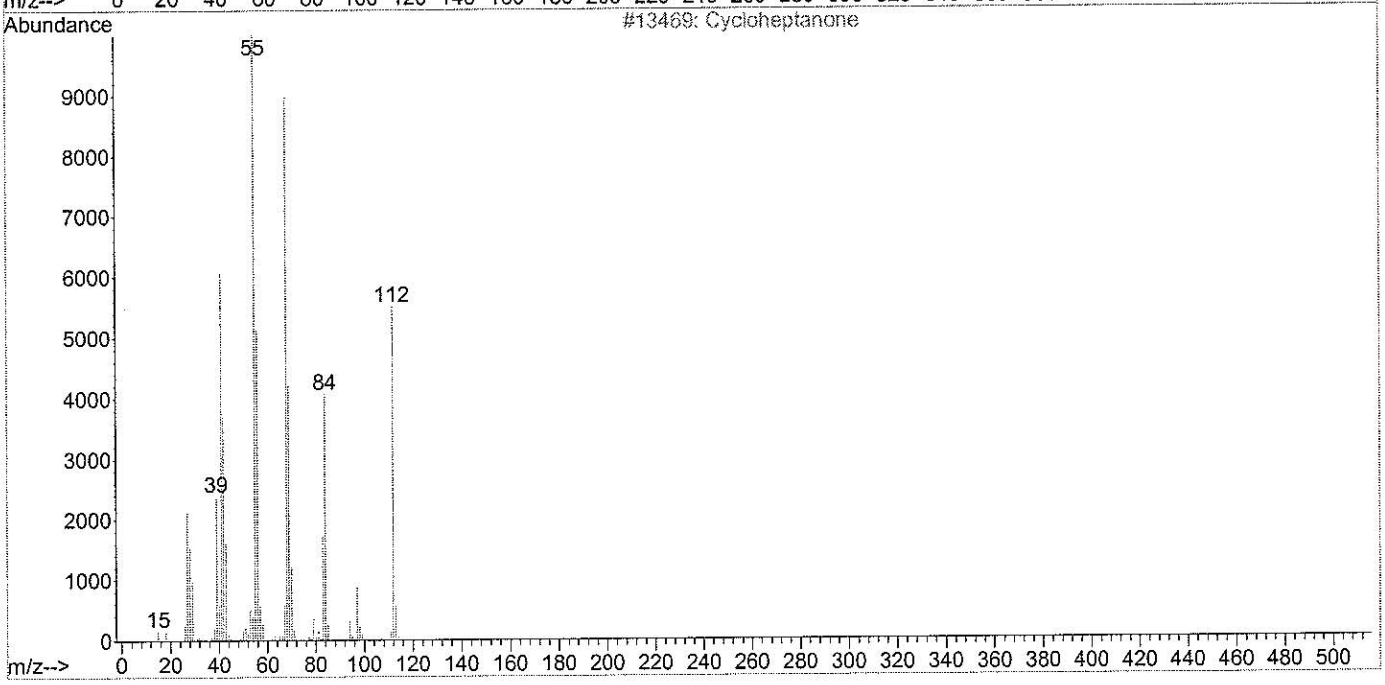

ac5033 e1 Jeyate CDCl3 a 4SPA 531
2c
175.2396
68.3039
33.5547
28.2772
27.9726
21.9184
(ppm)
220
200
180
160
140
120
100
80
60
40
20
0
BRUKER

CH. 1 C.S 10.00 ATT 3 OFFS 0 06/22/05 18:36

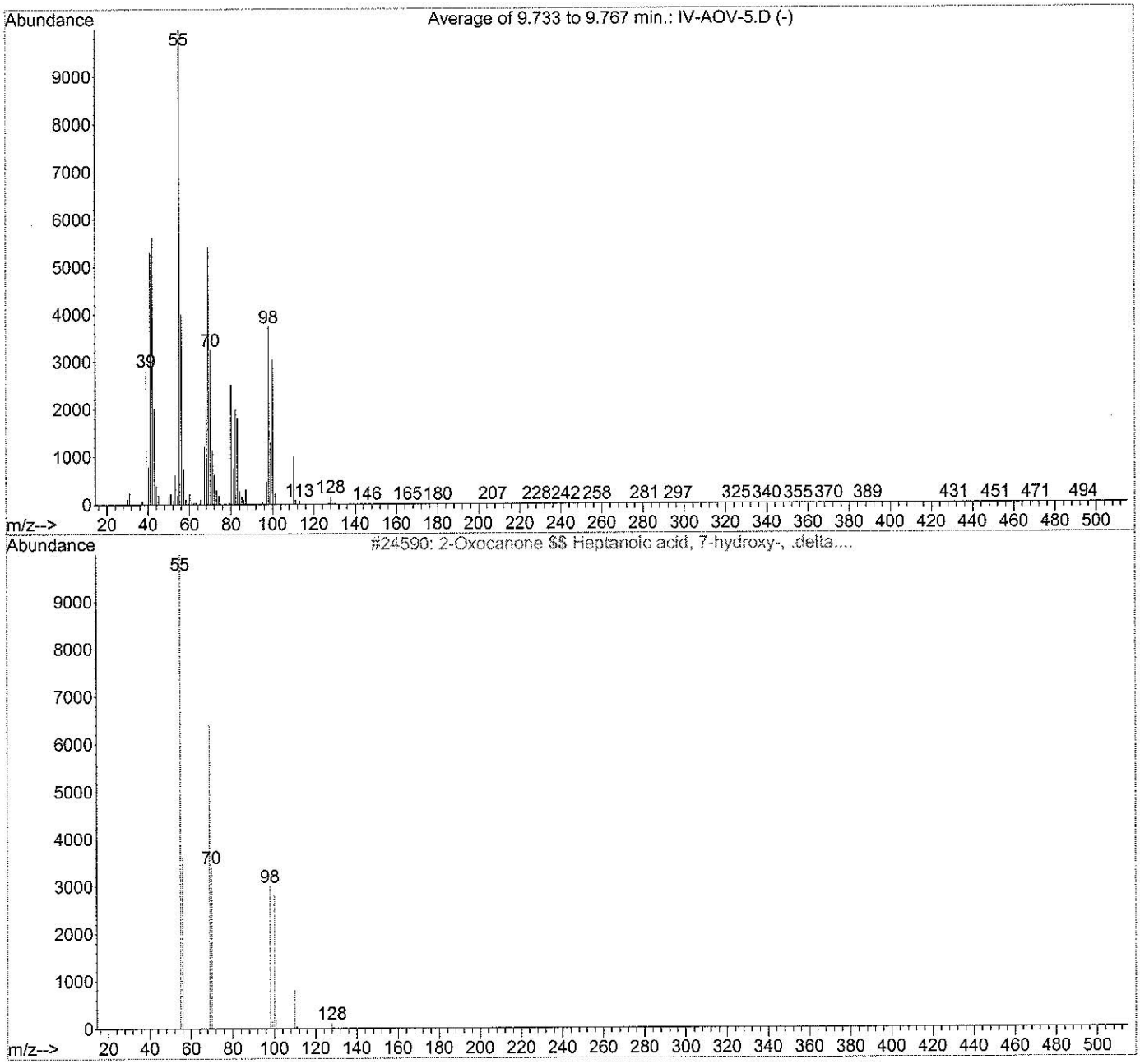


Library Searched : C:\DATABASE\wiley7n.L
Quality : 97
ID : Cycloheptanone

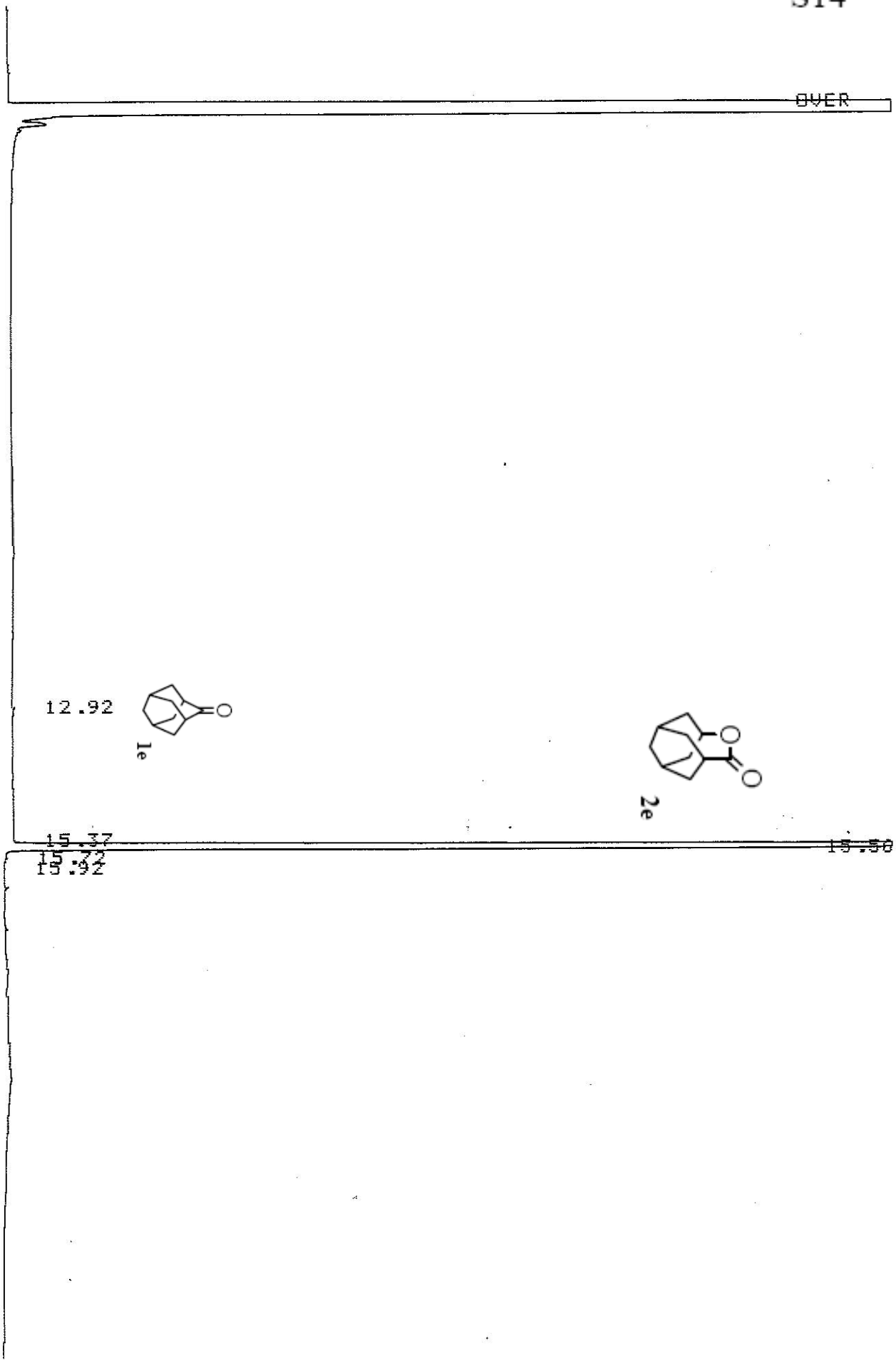




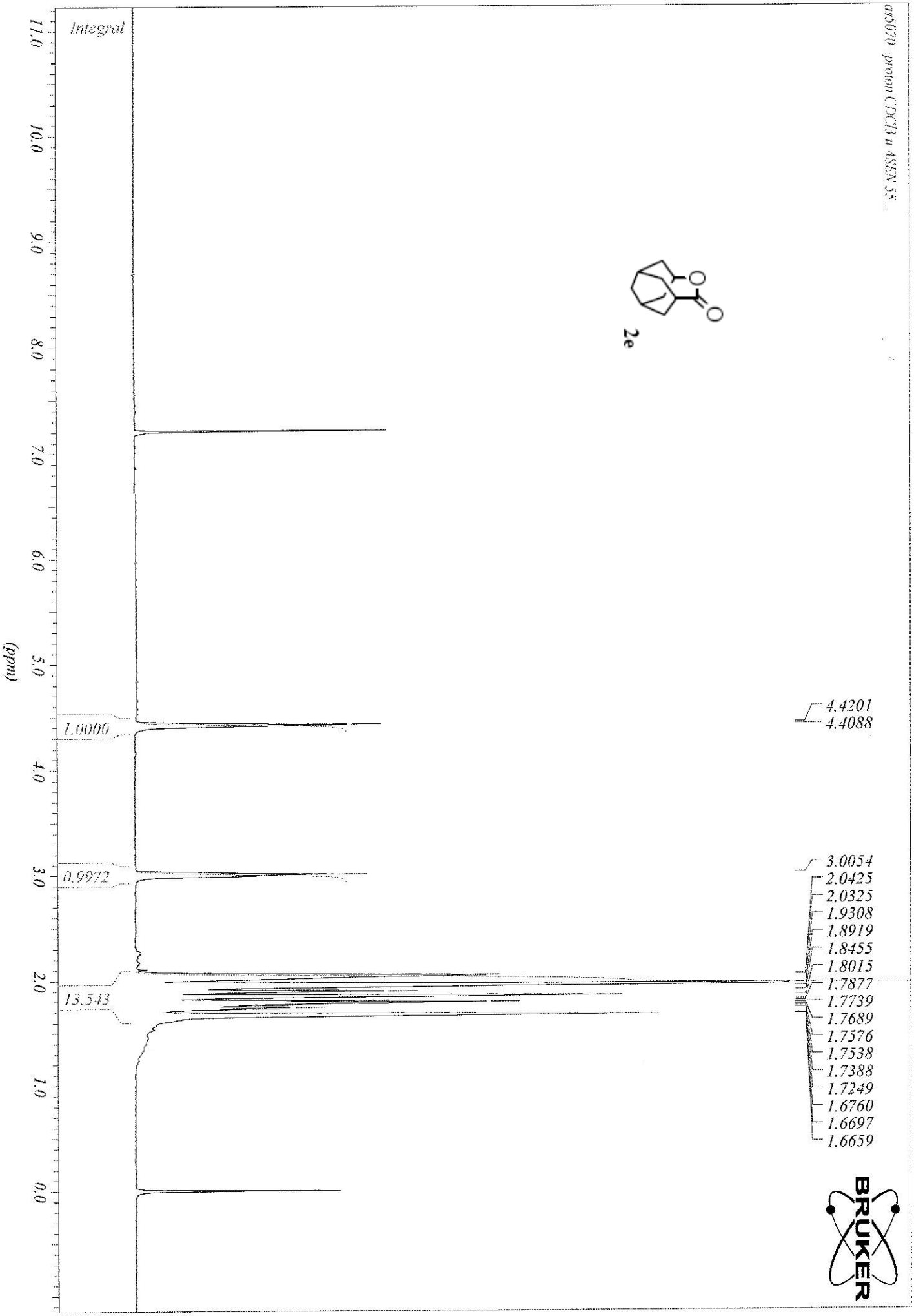
Library Searched : C:\DATABASE\wiley7n.L
Quality : 60
ID : 2-Oxocanone $$ Heptanoic acid, 7-hydroxy-, .delta.-lactone $$ .zeta .-Enantholactone $$ 1-Oxa-2-oxocyclooctane $$ Heptanoic acid, 7-hyd roxy-, .zeta.-lactone (CAS)



CH. 1 C.S 10.00 ATT 3 OFFS 0 12/14/05 16:30



D-2500 12/14/05 16:30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2e
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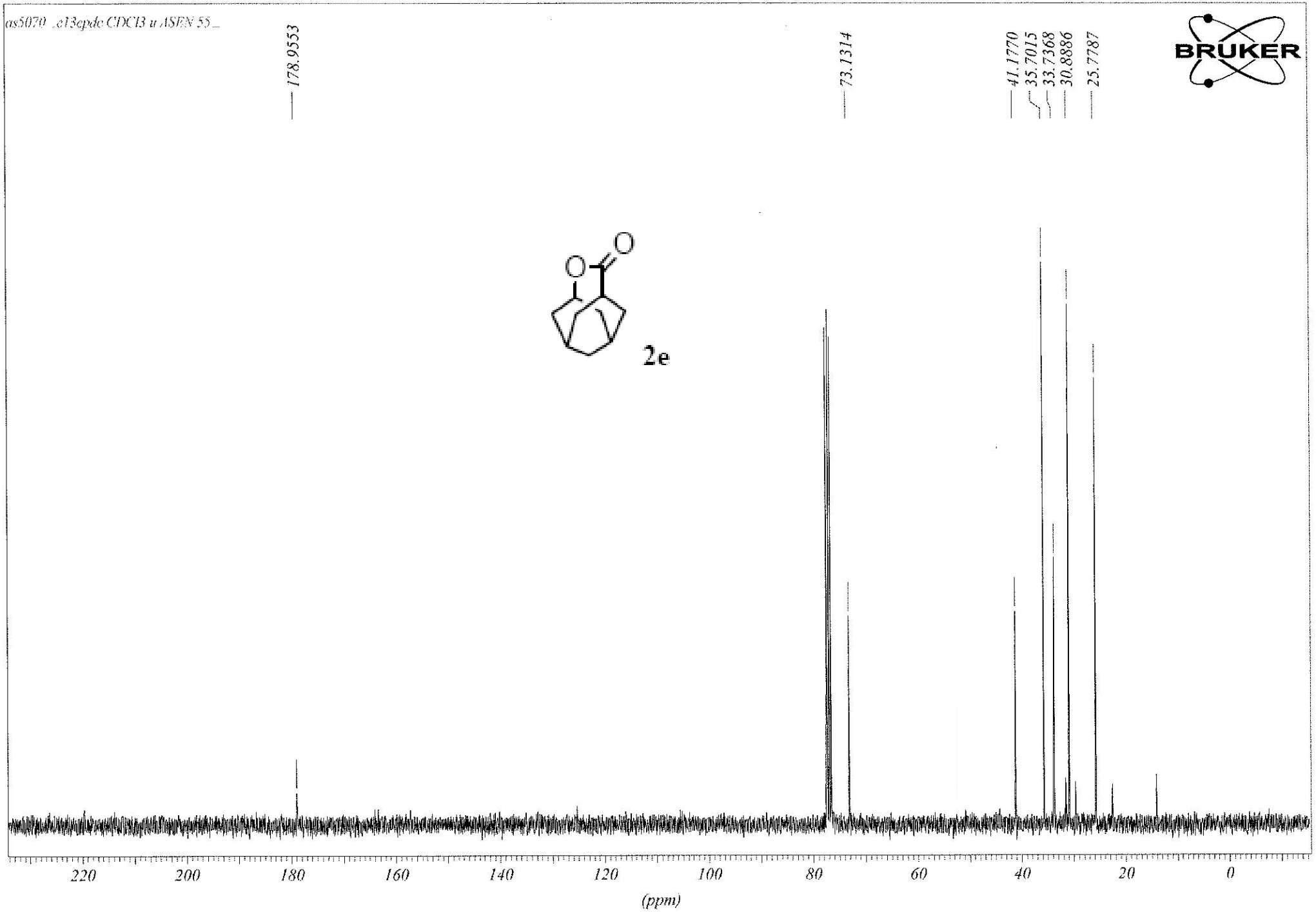
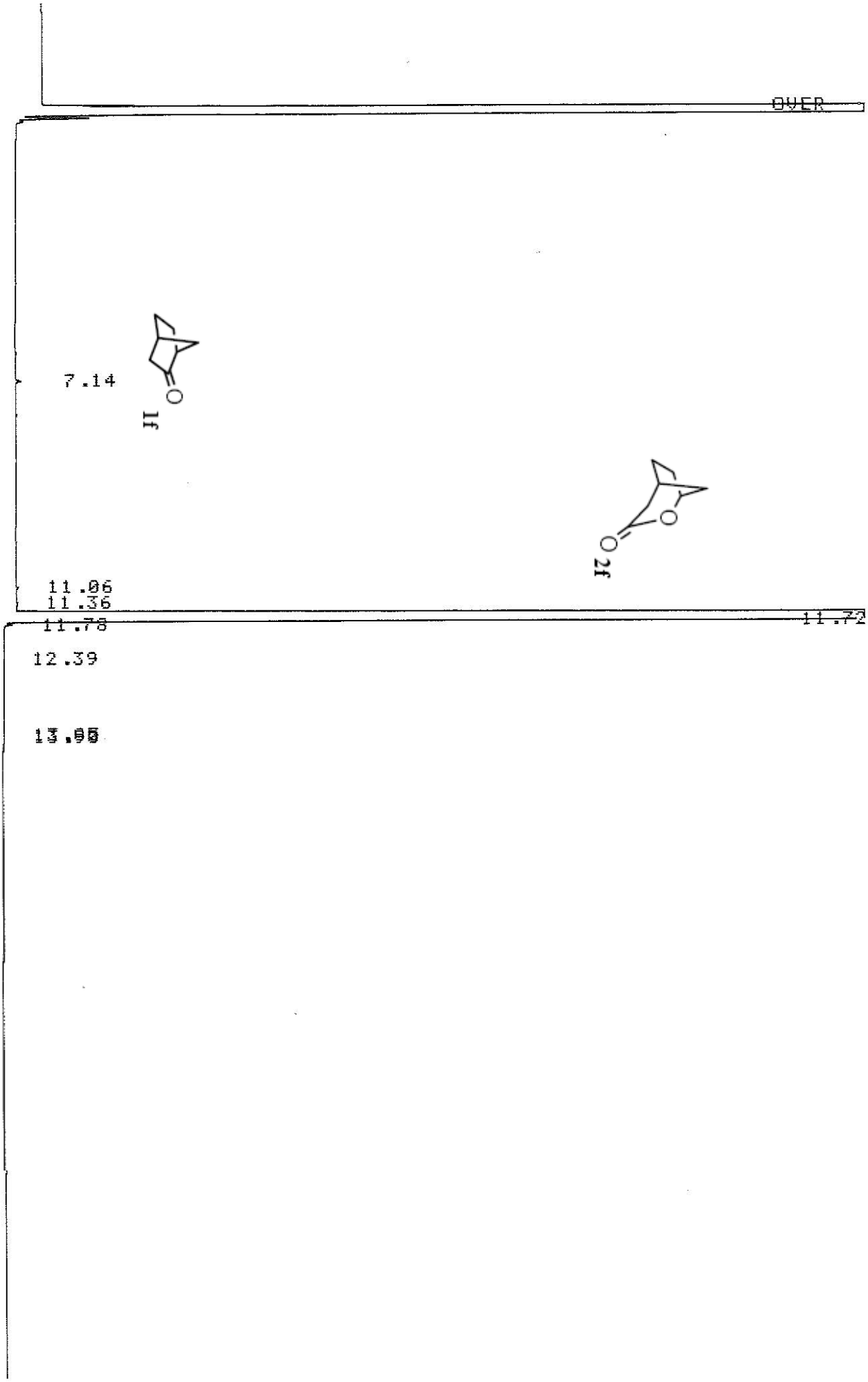
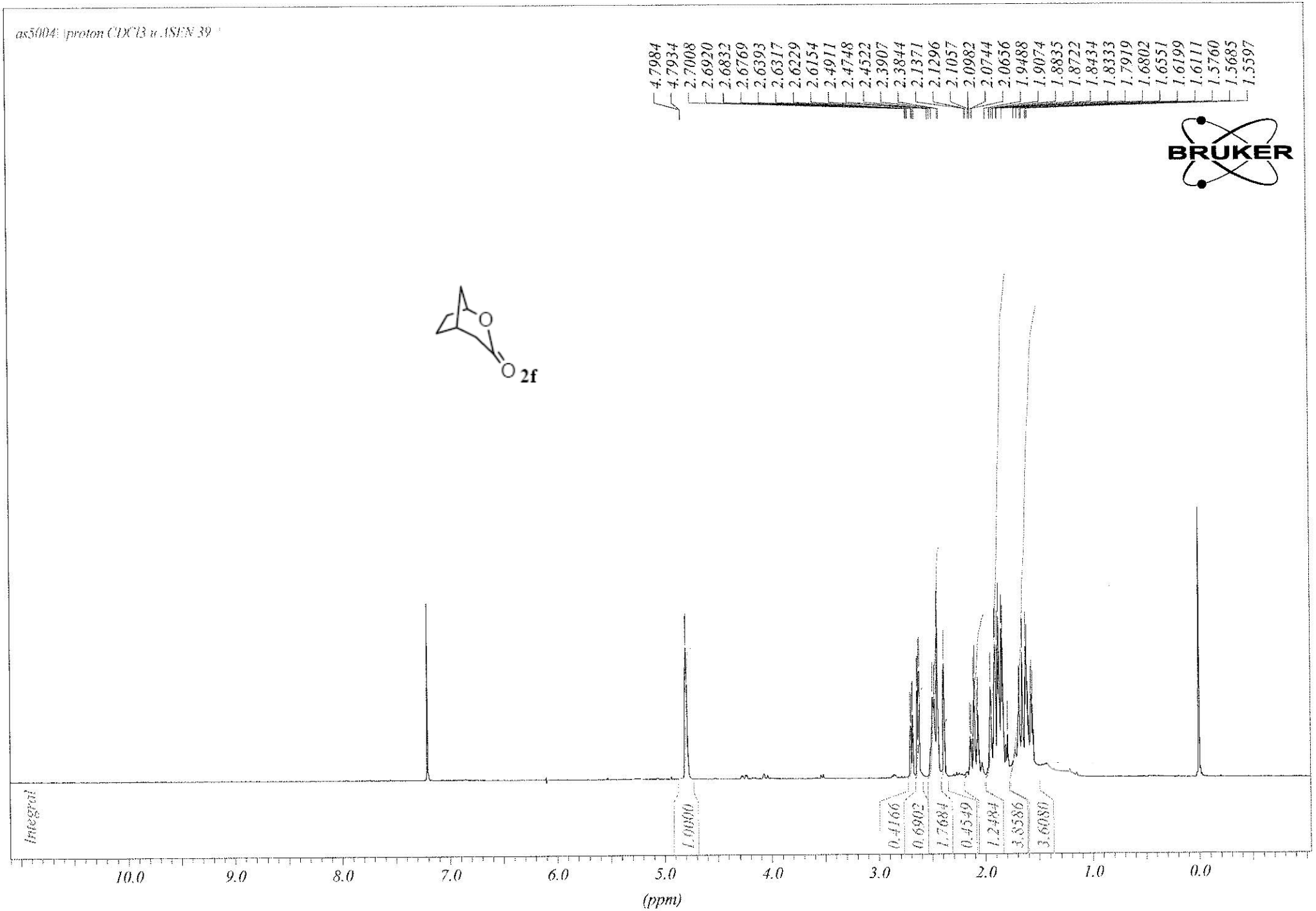
13.543
4.4201
4.4088
3.0054
2.0425
2.0325
1.9308
1.8919
1.8455
1.8015
1.7877
1.7739
1.7689
1.7576
1.7538
1.7388
1.7249
1.6760
1.6697
1.6659
(ppm)
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
BRUKER


as5070 _c13cpdc CDCl3 u ASEN 55 _
178.9553
73.1314
41.1770
35.7015
33.7368
30.8886
25.7787
BRUKER
2e
220
200
180
160
140
120
100
80
60
40
20
0
(ppm)

CH. 1 C.S 10.00 ATT 3 OFFS 0 10/11/05 13:08




as5004| |proton CDCl3 u ASEN 39
4.7984
4.7934
2.7008
2.6920
2.6832
2.6769
2.6393
2.6317
2.6229
2.6154
2.4911
2.4748
2.4522
2.3907
2.3844
2.1371
2.1296
2.1057
2.0982
2.0744
2.0656
1.9488
1.9074
1.8835
1.8722
1.8434
1.8333
1.7919
1.6802
1.6551
1.6199
1.6111
1.5760
1.5685
1.5597
BRUKER
2f
1.0000
0.4166
0.6902
1.7684
0.4549
1.2484
3.8586
3.6080
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1.0
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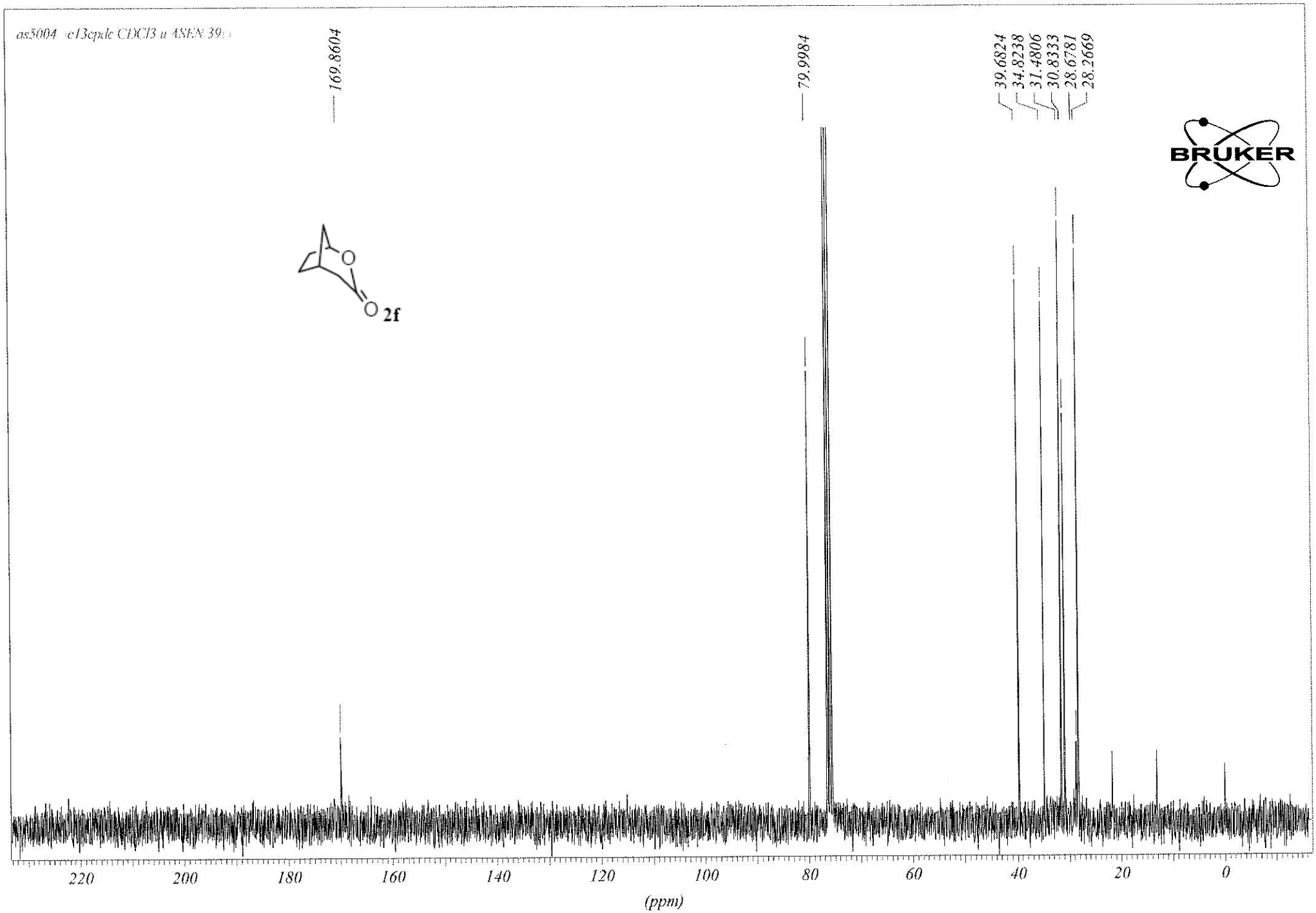
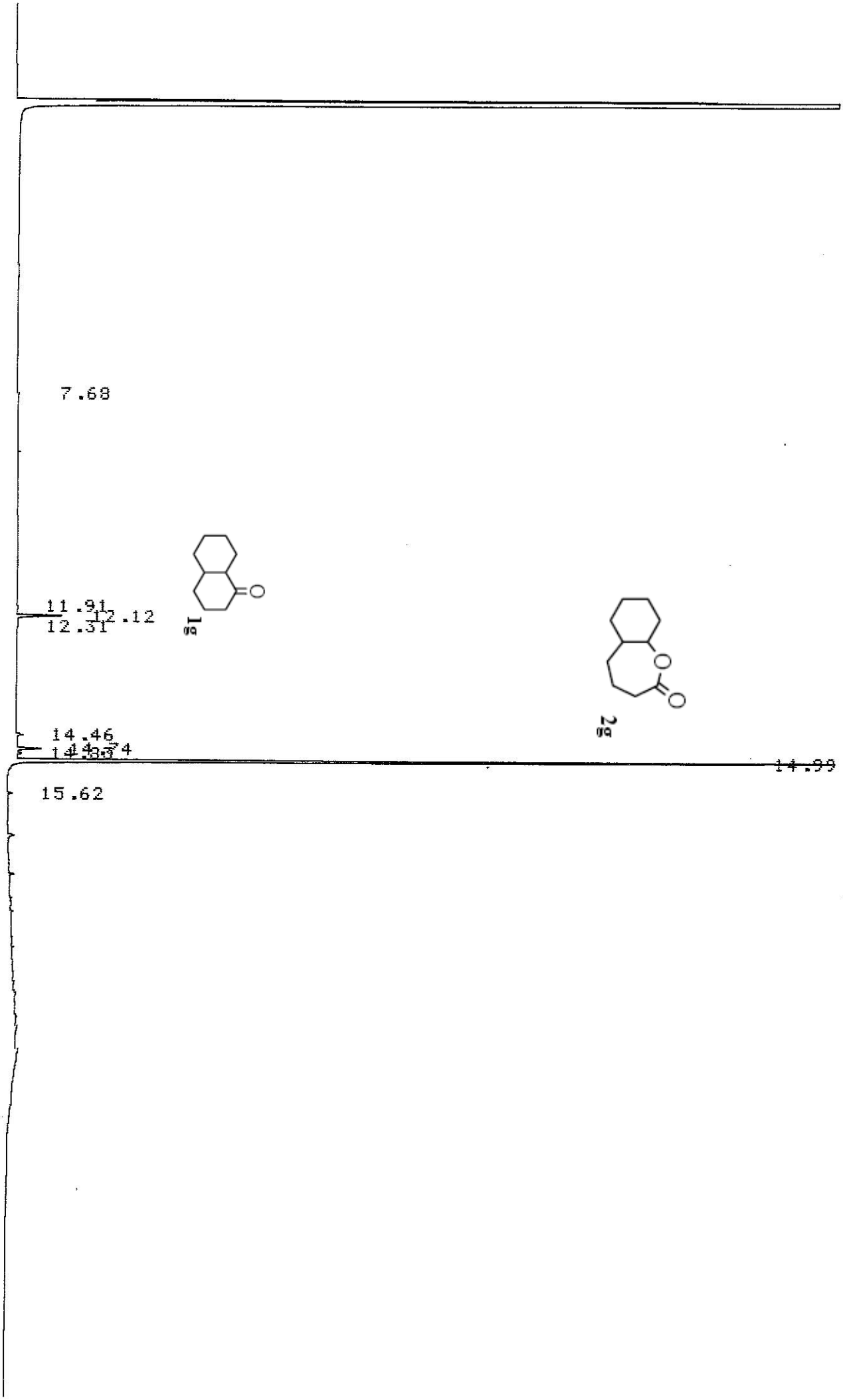
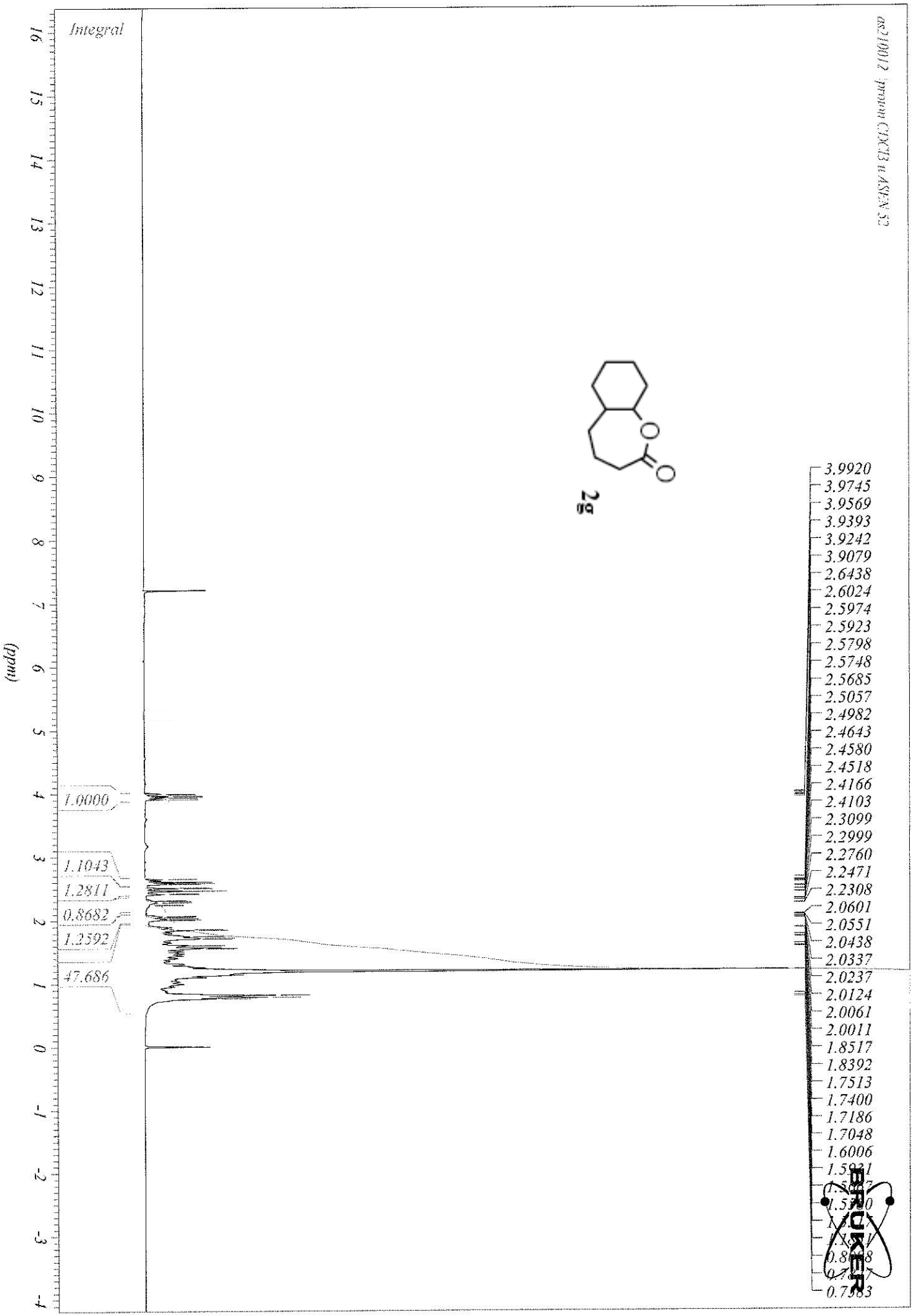
(ppm)


as5004 c13cpdc CDCl3 u 4SEN 39
169.8604
79.9984
39.6824
34.8238
31.4806
30.8333
28.6781
28.2669
2f
BRUKER
220
200
180
160
140
120
100
80
60
40
20
0
(ppm)

CH. 1 C.S 10.00 ATT 3 OFFS 0 01/12/06 14:03

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3.9745
3.9569
3.9393
3.9242
3.9079
2.6438
2.6024
2.5974
2.5923
2.5798
2.5748
2.5685
2.5057
2.4982
2.4643
2.4580
2.4518
2.4166
2.4103
2.3099
2.2999
2.2760
2.2471
2.2308
2.0601
2.0551
2.0438
2.0337
2.0237
2.0124
2.0061
2.0011
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1.8392
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1.7048
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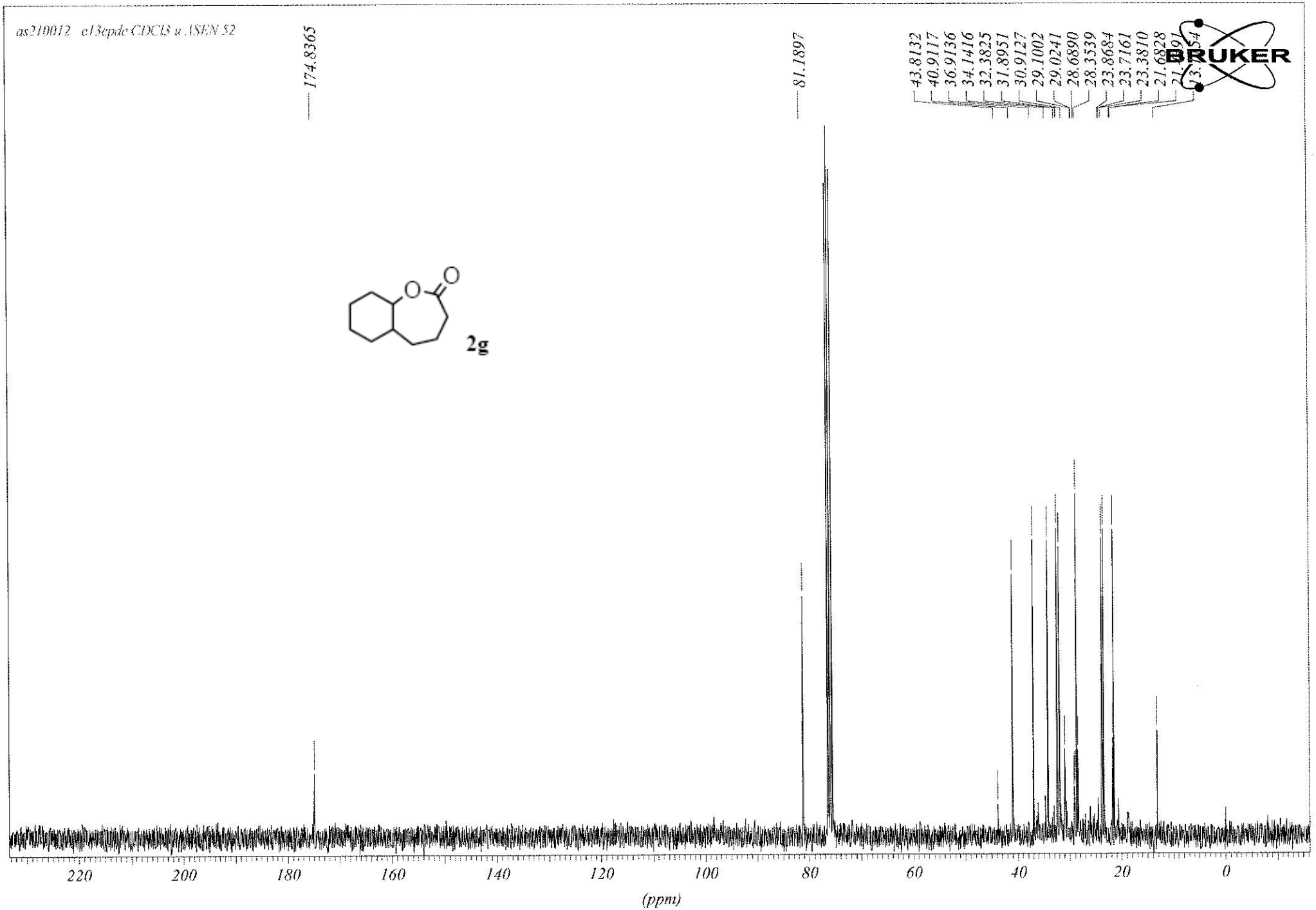
(ppm)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43.8132
40.9117
36.9136
34.1416
32.3825
31.8951
30.9127
29.1002
29.0241
28.6890
28.3539
23.8684
23.7161
23.3810
21.6828
21.6891
13.7154
BRUKER
2g
220
200
180
160
140
120
100
80
60
40
20
0
(ppm)

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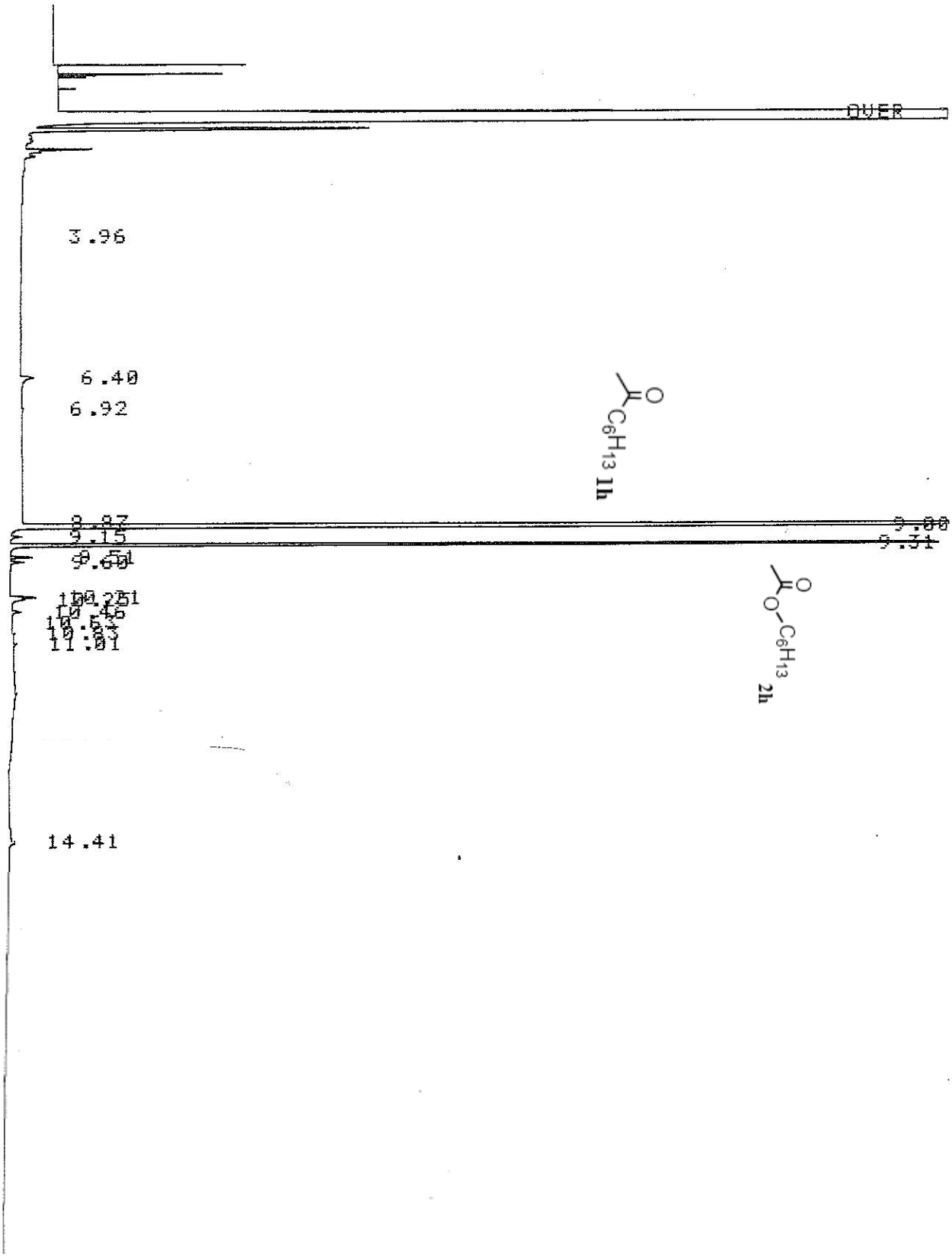

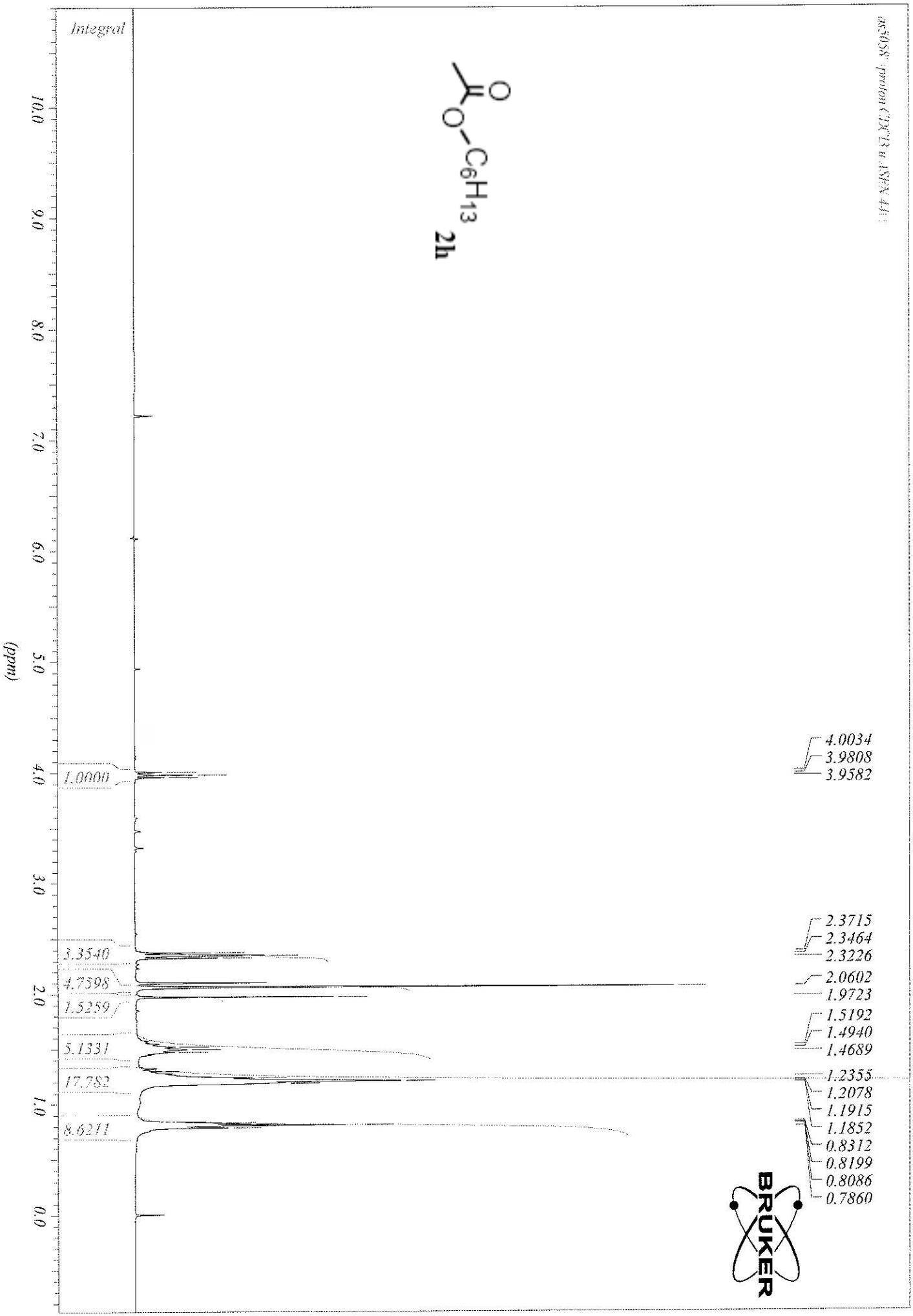
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2h
Integral
(ppm)
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7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
1.0000
3.3540
4.7598
1.5259
5.1331
17.782
8.6211
4.0034
3.9808
3.9582
2.3715
2.3464
2.3226
2.0602
1.9723
1.5192
1.4940
1.4689
1.2355
1.2078
1.1915
1.1852
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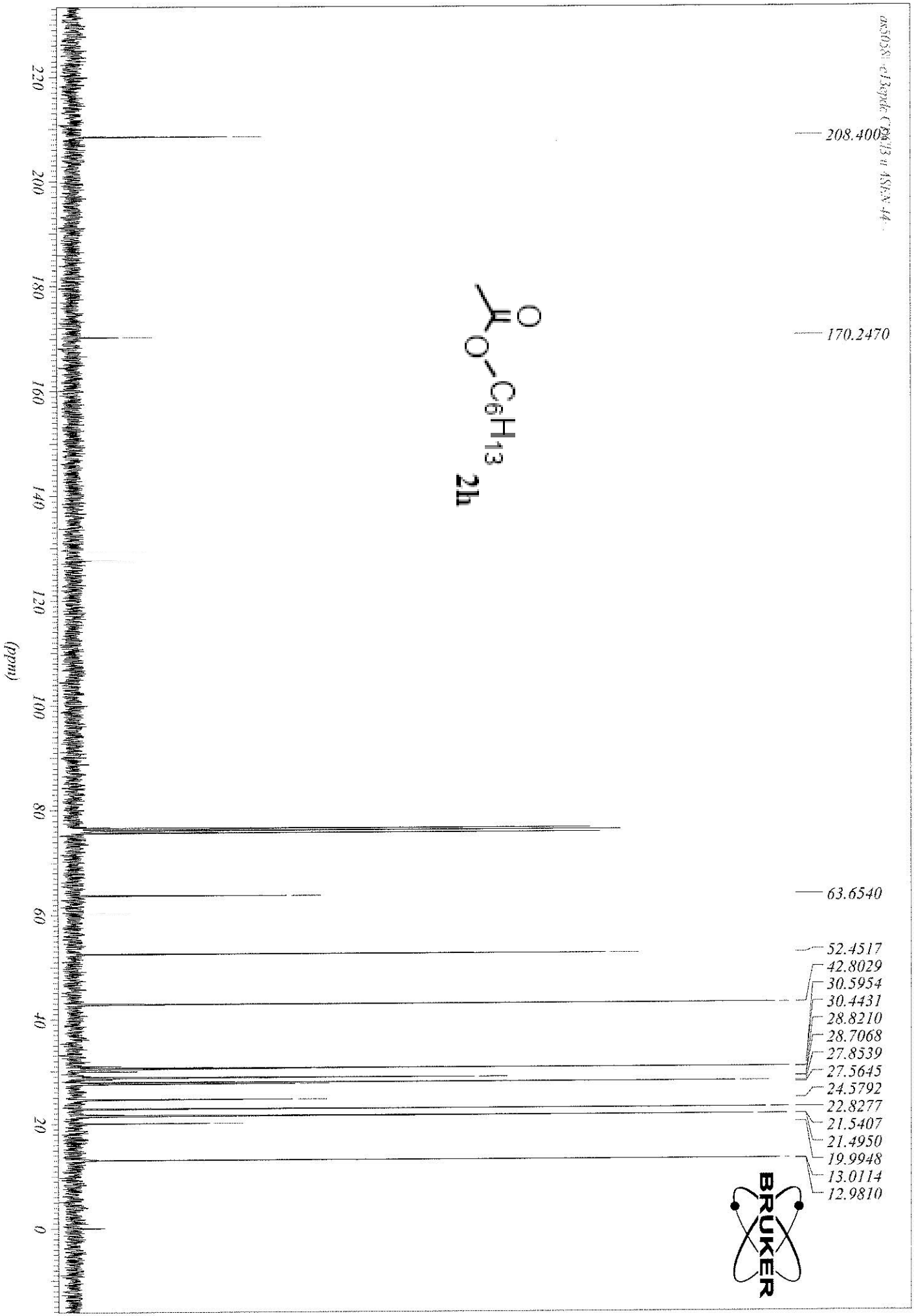
0.8199
0.8086
0.7860
BRUKER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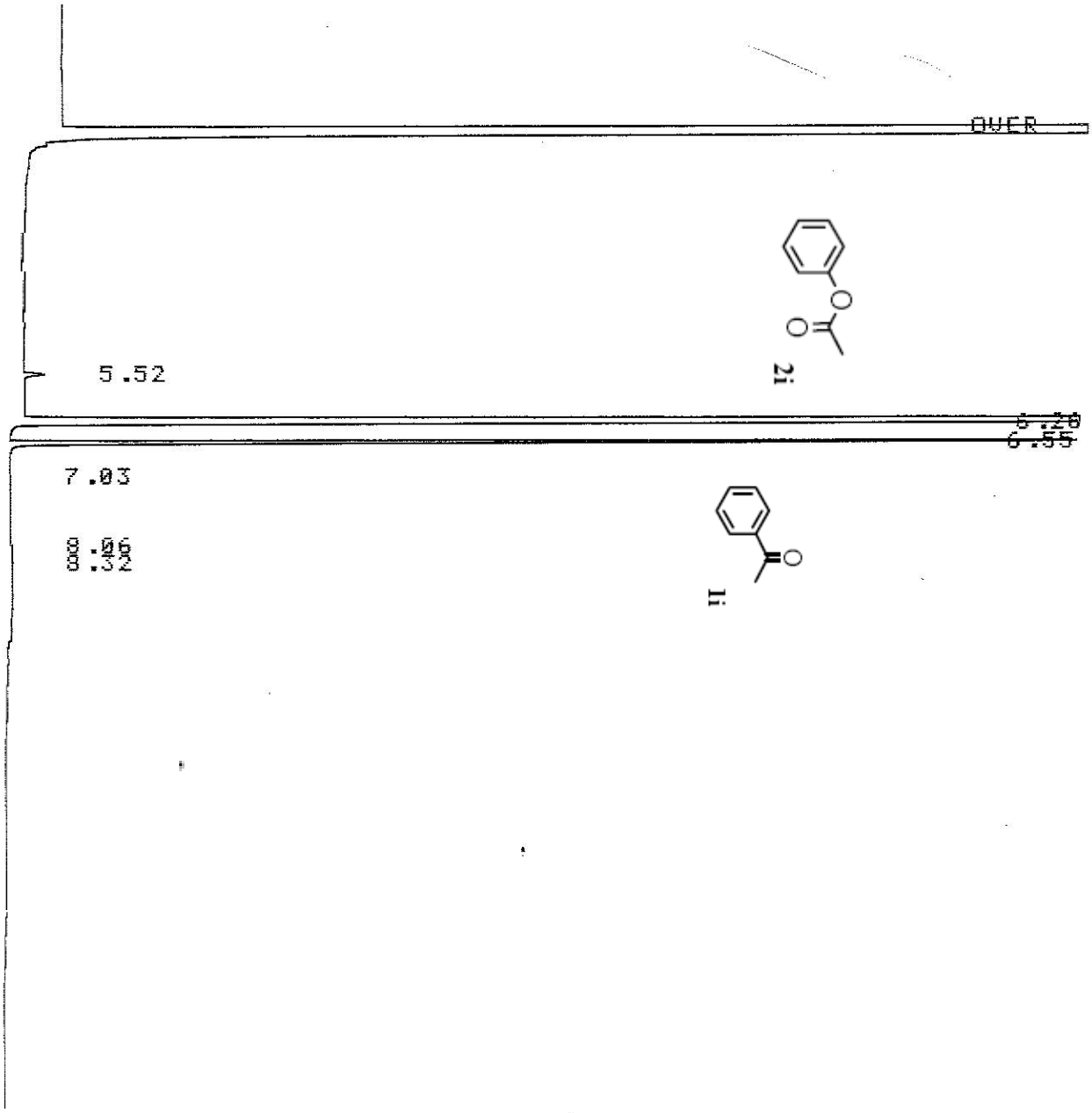
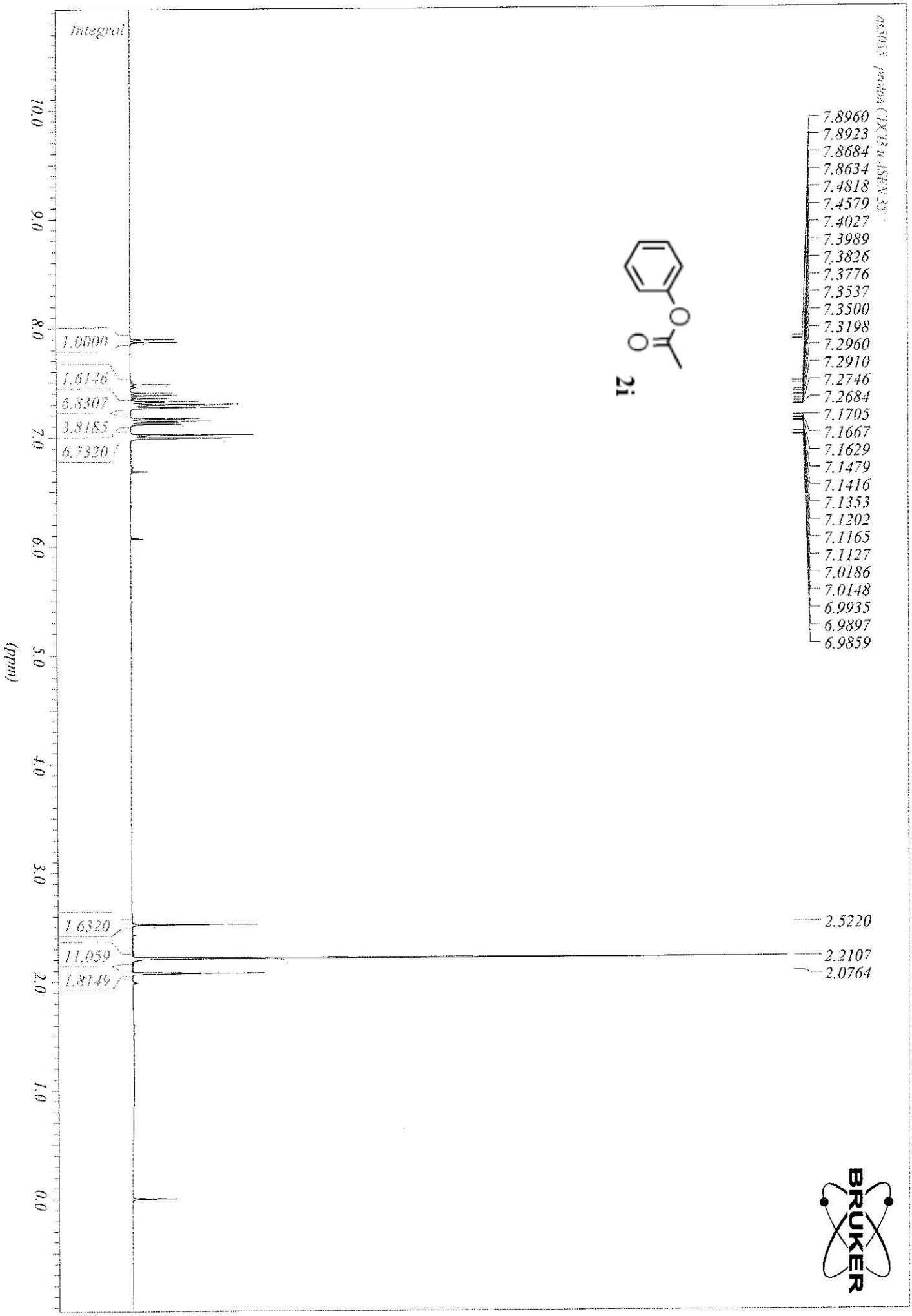
208.4000
170.2470
63.6540
52.4517
42.8029
30.5954
30.4431
28.8210
28.7068
27.8539
27.5645
24.5792
22.8277
21.5407
21.4950
19.9948
13.0114
12.9810
220
200
180
160
140
120
100
80
60
40
20
0
(ppm)
O
O
C6H13
2h
BRUKER

CH. 1 C.S 10.00 ATT 3 OFFS 0 11/16/05 13:38




Integral
(ppm)
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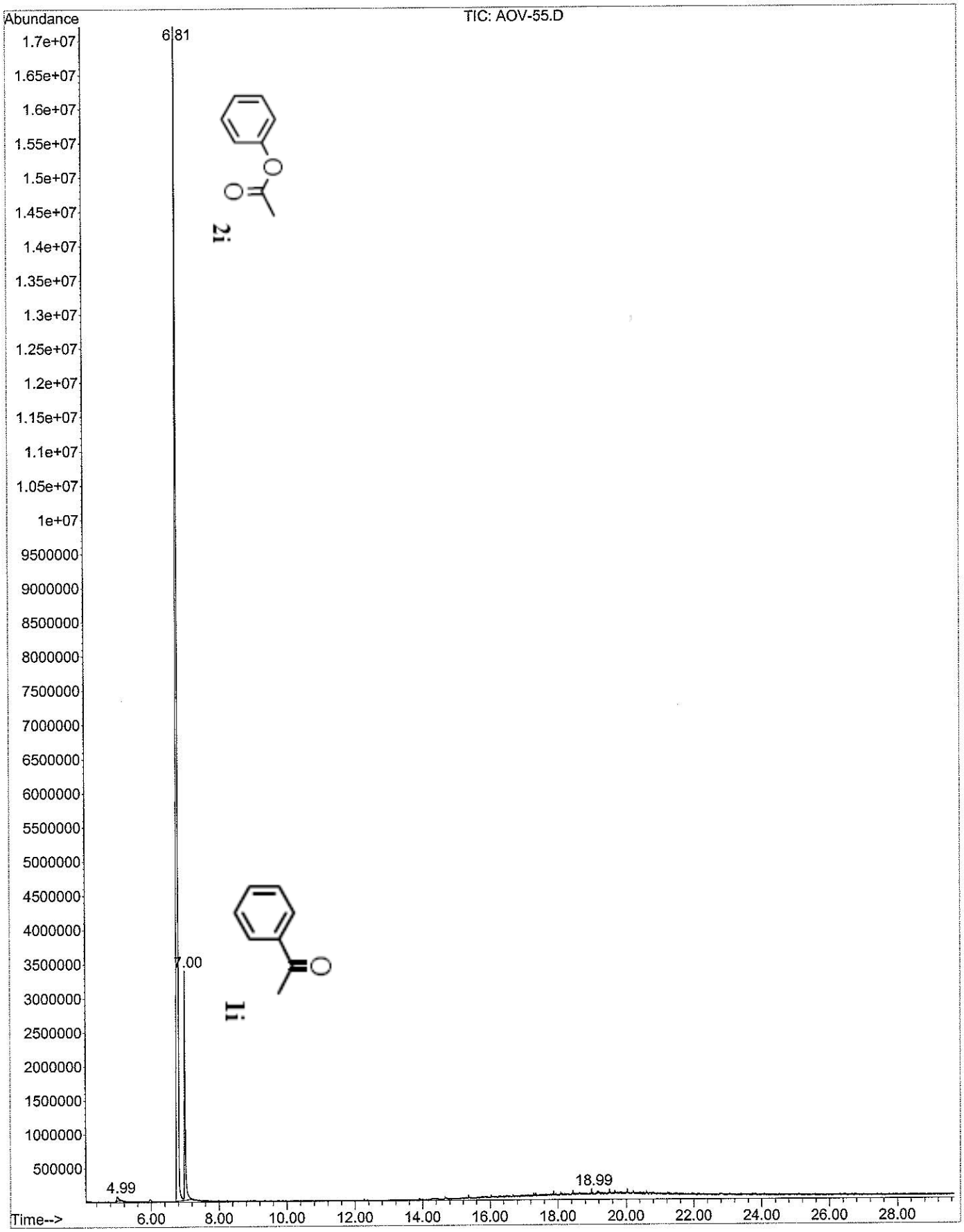
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
1.0000
1.6146
6.8307
3.8185
6.7320
1.6320
11.059
1.8149
7.8960
7.8923
7.8684
7.8634
7.4818
7.4579
7.4027
7.3989
7.3826
7.3776
7.3537
7.3500
7.3198
7.2960
7.2910
7.2746
7.2684
7.1705
7.1667
7.1629
7.1479
7.1416
7.1353
7.1202
7.1165
7.1127
7.0186
7.0148
6.9935
6.9897
6.9859
2.5220
2.2107
2.0764
2i
BRUKER

Area Percent Report

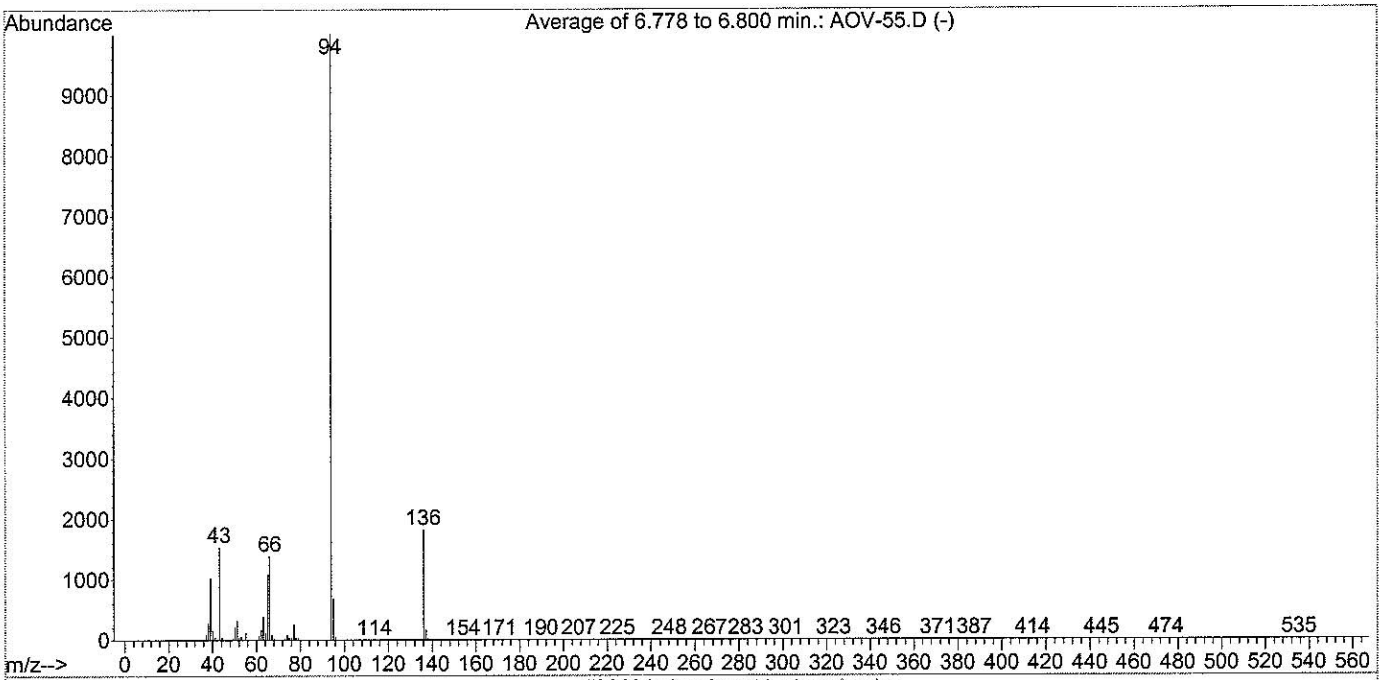
Data File : C:\MSDCHEM\1\DATA\JPEREZ\MAICA\AOV-55.D
Acq On : 18 Nov 2005 15:11
Sample :
Misc :

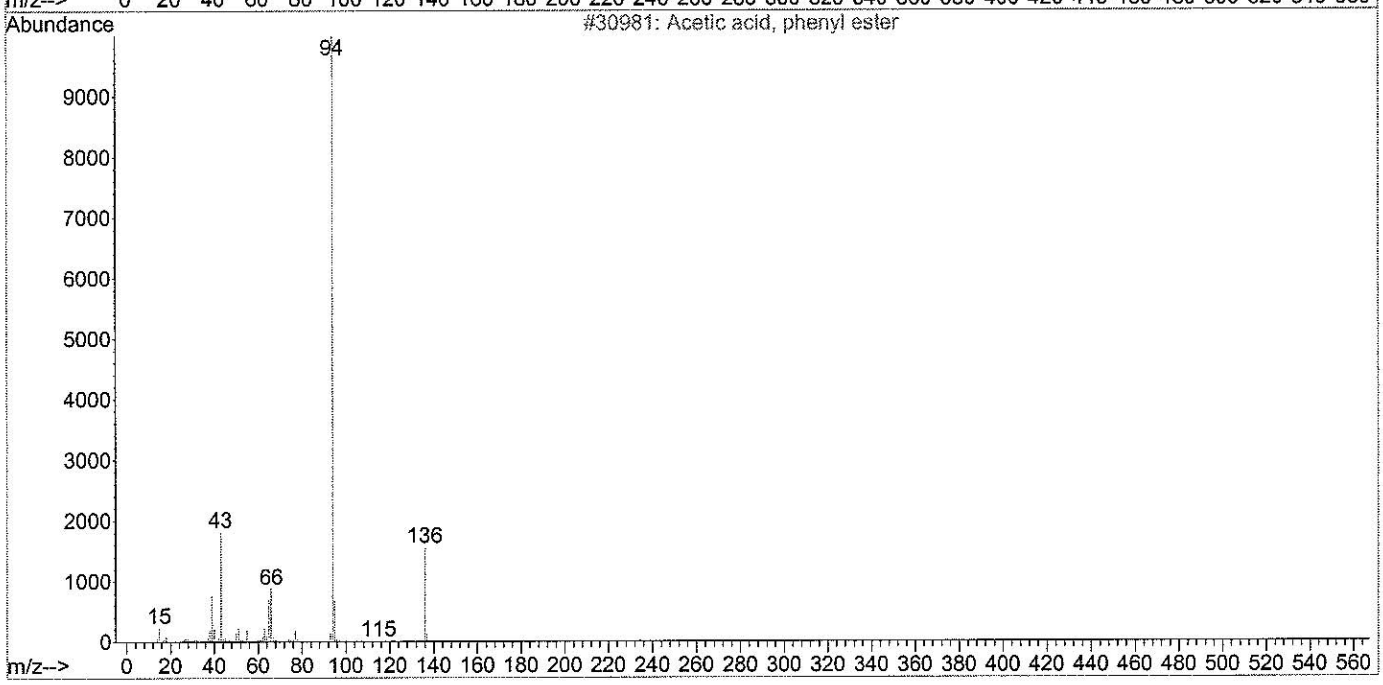
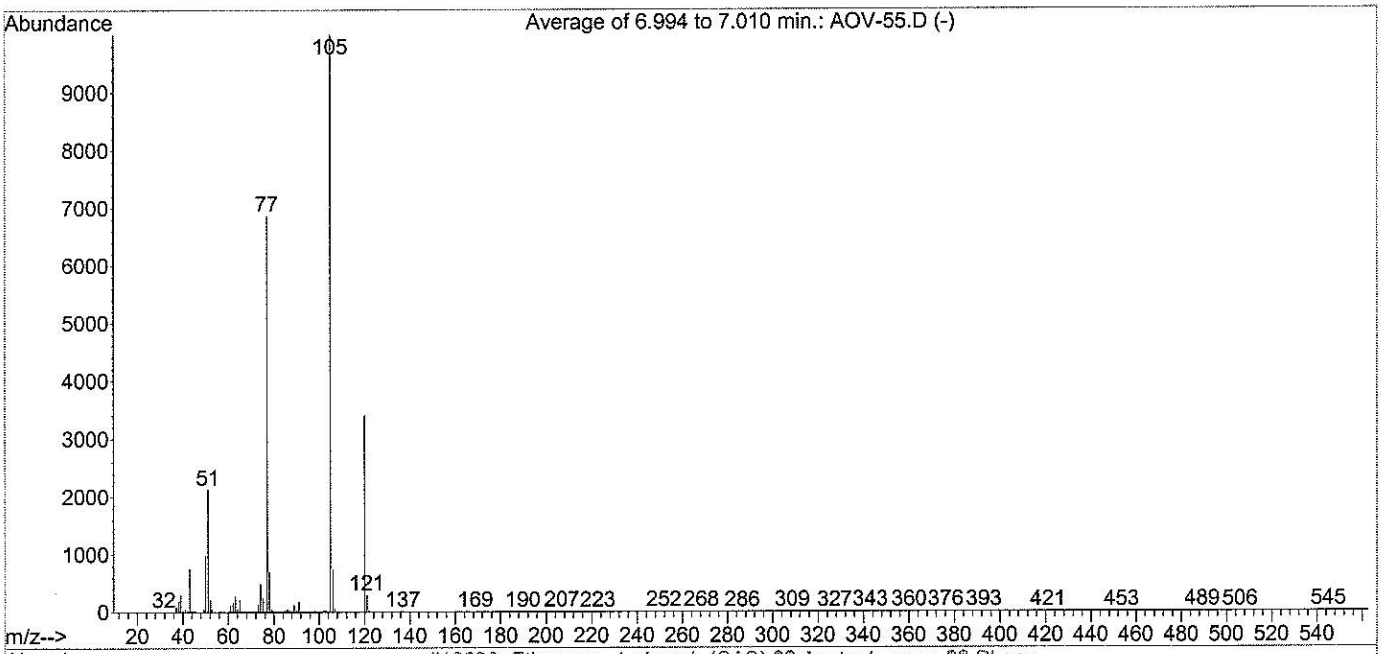
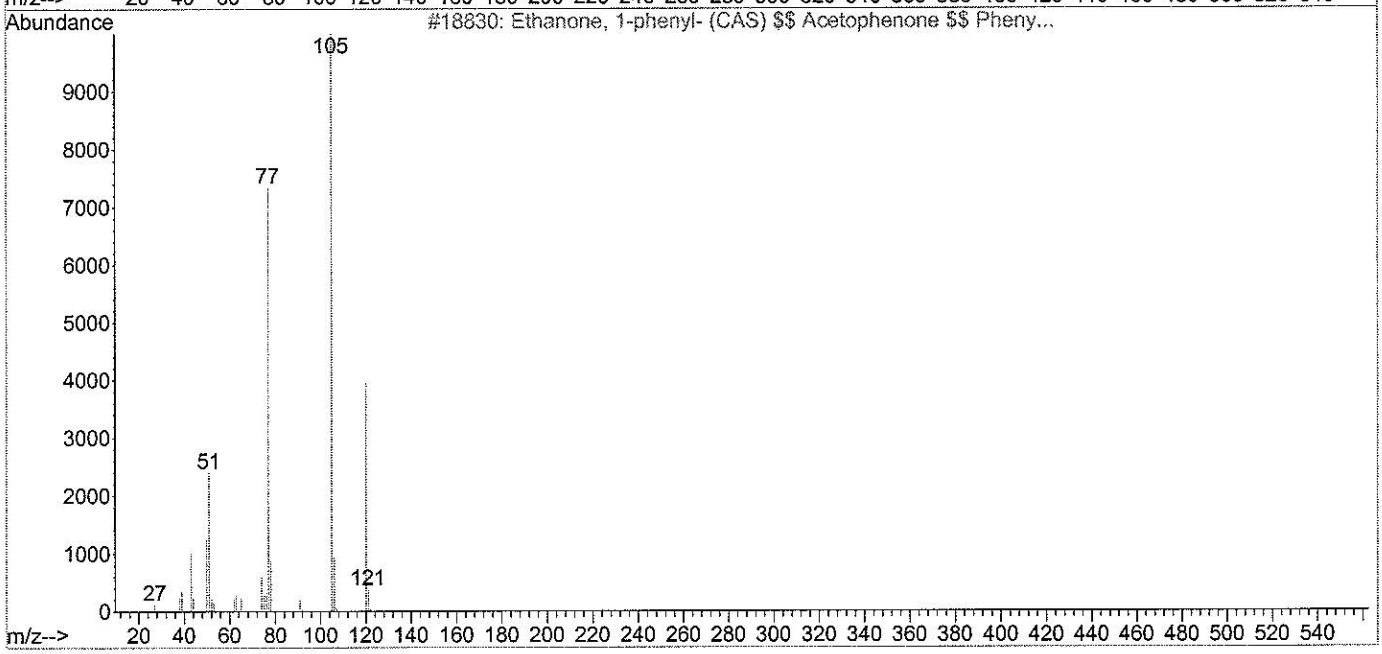
Vial: 9
Operator: maica
Inst : Instrumen
Multiplr: 1.00
Sample Amount: 0.00

MS Integration Params: AUTOINT1.E
Method : C:\MSDCHEM\1\METHODS\AND.M (Chemstation Integrator)
Title :



Library Searched : C:\DATABASE\wiley7n.L
Quality : 91
ID : Acetic acid, phenyl ester

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