

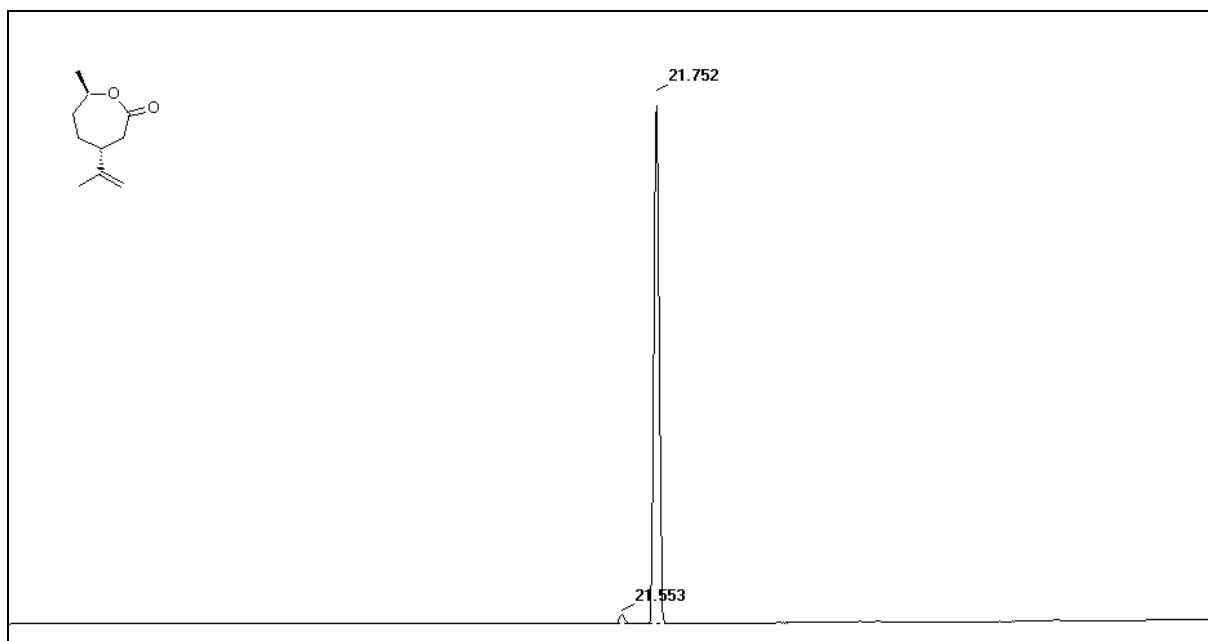
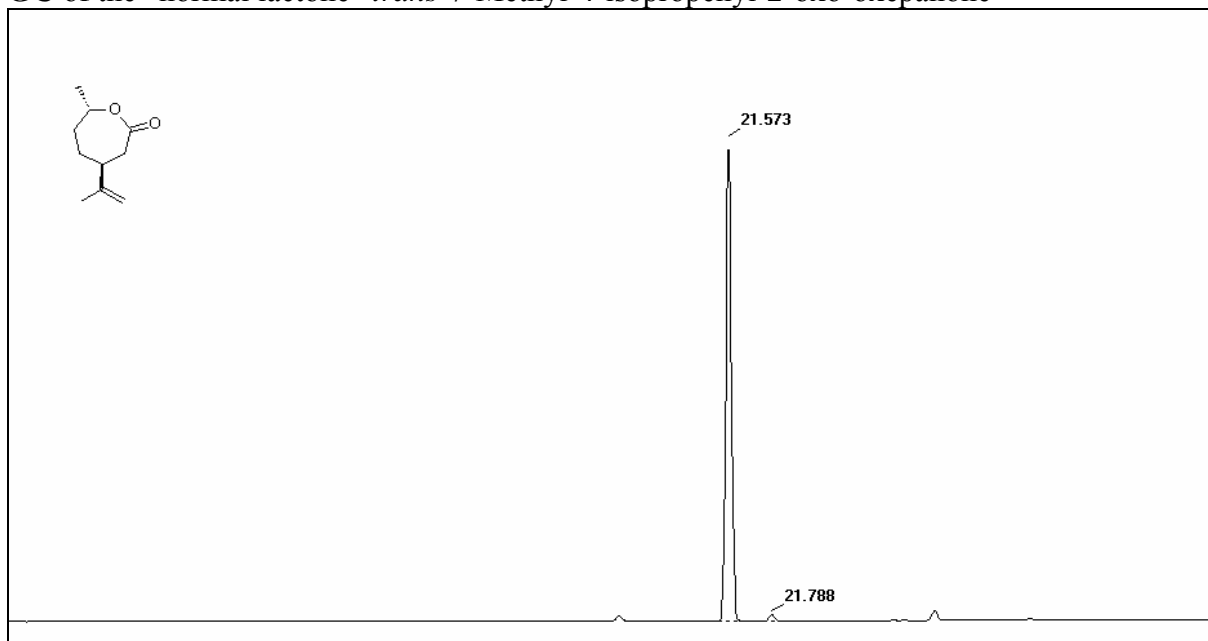
# Supplementary Data

Microbial Baeyer-Villiger Oxidation of Terpenones by Recombinant Whole-Cell Biocatalysts – Formation of Enantiocomplementary Regioisomeric Lactones.

Petra Černuchová and Marko D. Mihovilovic

*Institute of Applied Synthetic Chemistry, Vienna University of Technology, Getreidemarkt 9/163-OC, 1060 Vienna, Austria.  
Fax: +43-1-58801-15499; Tel.: +43-1-58801-15420;  
E-mail: mmihovil@pop.tuwien.ac.at*

GC of the "normal lactone" *trans*-7-Methyl-4-isopropenyl-2-oxo-oxepanone



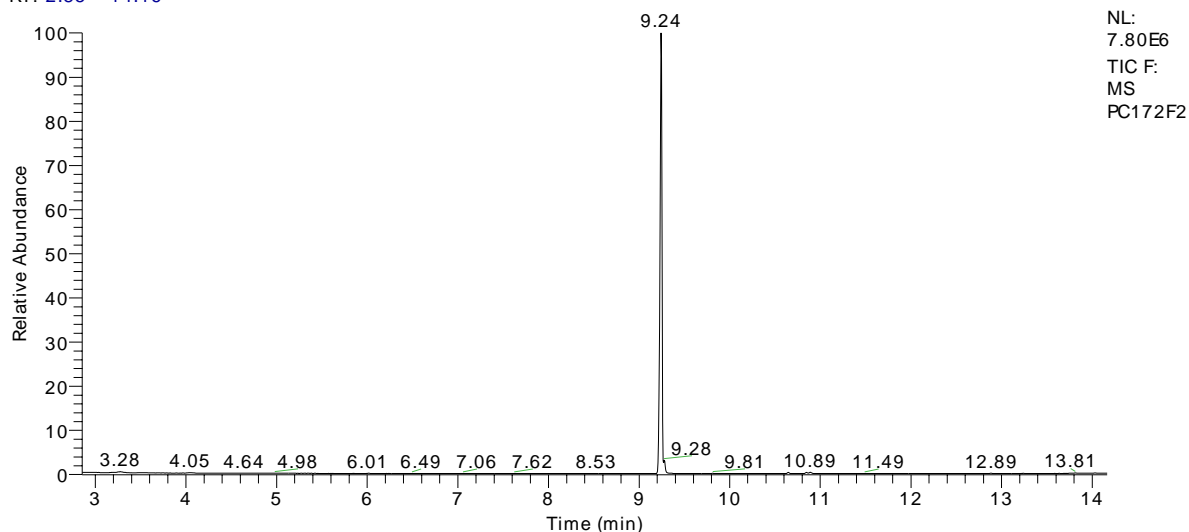
# GC MS of the "normal lactone" *trans*-7-Methyl-4-isopropenyl-2-oxo-oxepanone

D:\Dokumenty\viaden\GCMS\PC172F2

12. 9. 2006 20:01:15

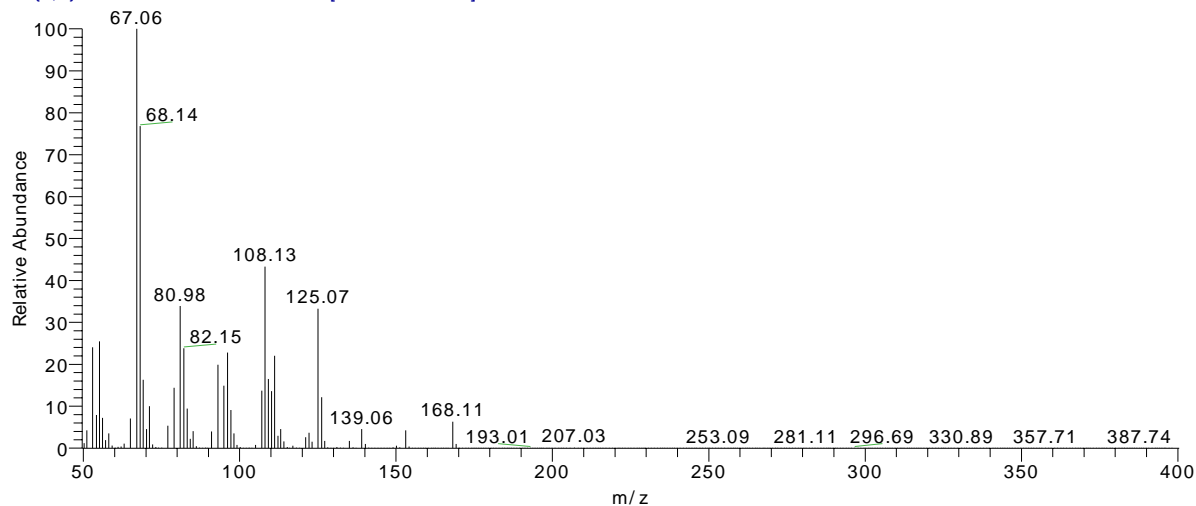
PC172F2

RT: 2.85 - 14.16



PC172F2 #1302-1307 RT: 9.22-9.25 AV: 6 NL: 8.17E5

T: {0;0} + c EI det=350.00 Full ms [ 50.00-400.00]



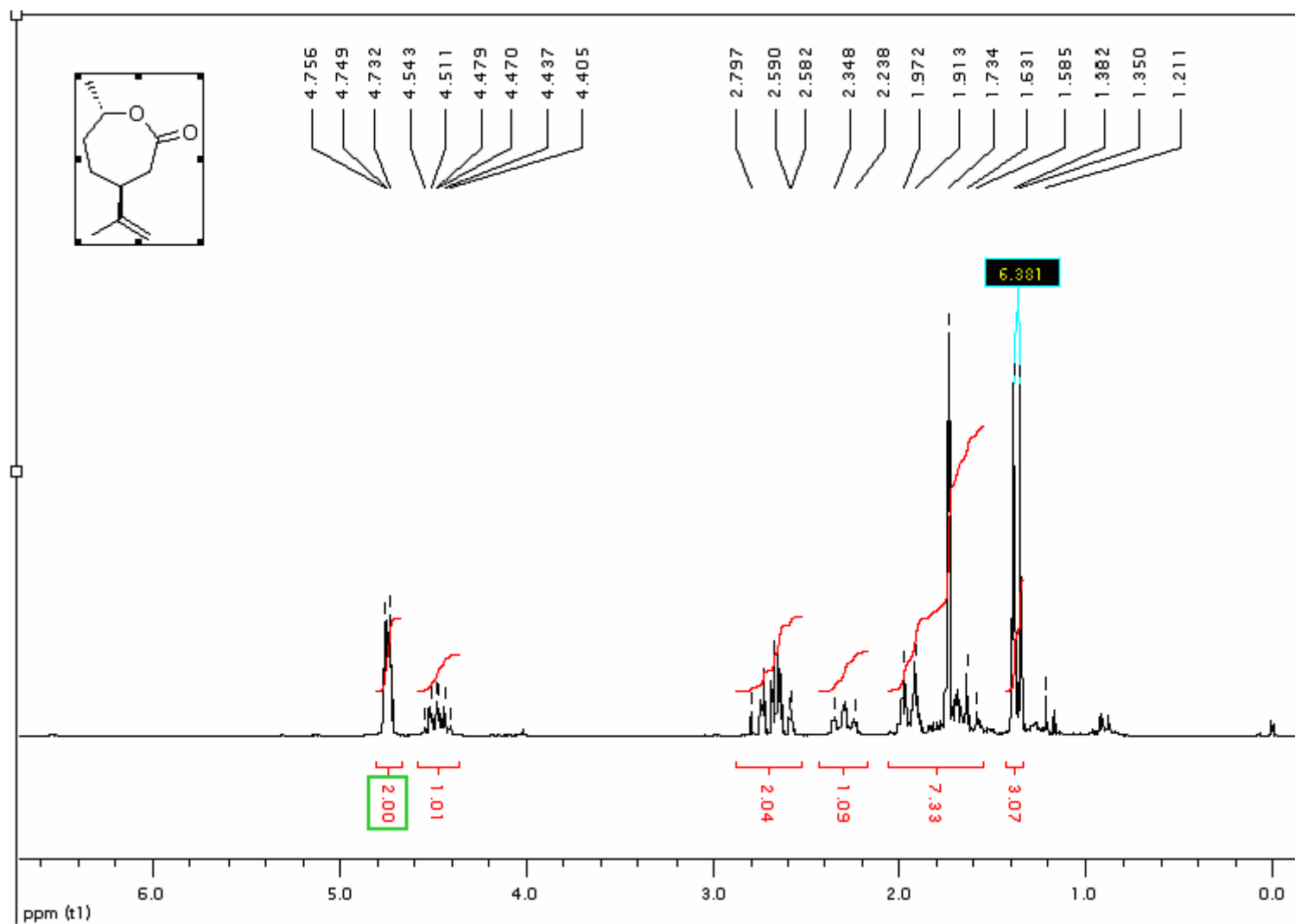
PC172F2#1302-1307 RT: 9.22-9.25 AV: 6

T: {0;0} + c EI det=350.00 Full ms [ 50.00-400.00]

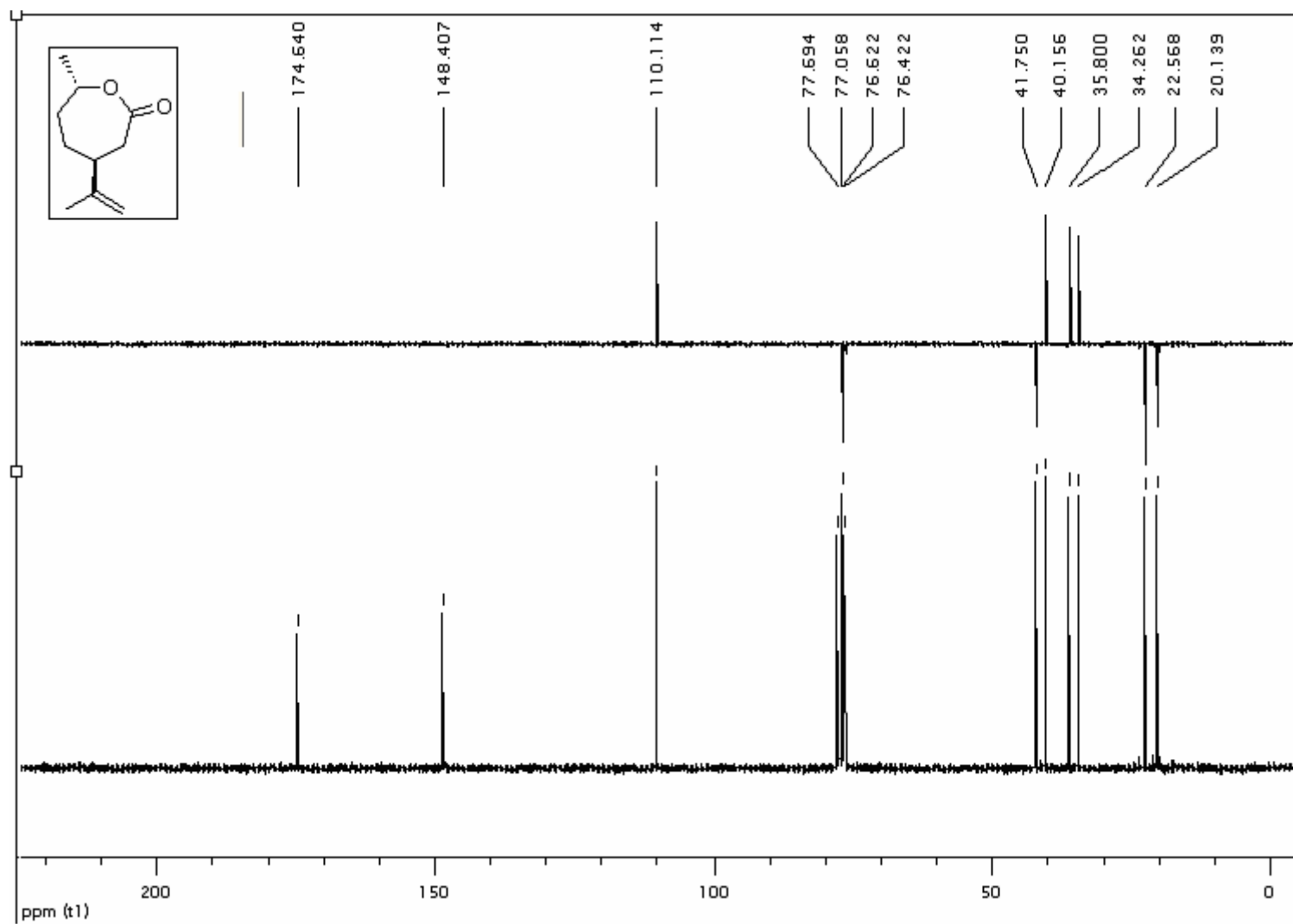
m/z= 49.60-400.40

| m/z    | Intensity | Relative |
|--------|-----------|----------|
| 52.95  | 196120.0  | 24.02    |
| 55.12  | 207610.7  | 25.43    |
| 67.06  | 816501.3  | 100.00   |
| 68.14  | 626634.7  | 76.75    |
| 69.16  | 132645.3  | 16.25    |
| 71.10  | 81090.7   | 9.93     |
| 79.00  | 117045.3  | 14.33    |
| 80.98  | 276405.3  | 33.85    |
| 82.15  | 194234.7  | 23.79    |
| 83.16  | 76573.3   | 9.38     |
| 93.03  | 162240.0  | 19.87    |
| 94.96  | 121290.7  | 14.85    |
| 96.12  | 185752.0  | 22.75    |
| 107.06 | 111520.0  | 13.66    |
| 108.13 | 352885.3  | 43.22    |
| 109.18 | 133970.7  | 16.41    |

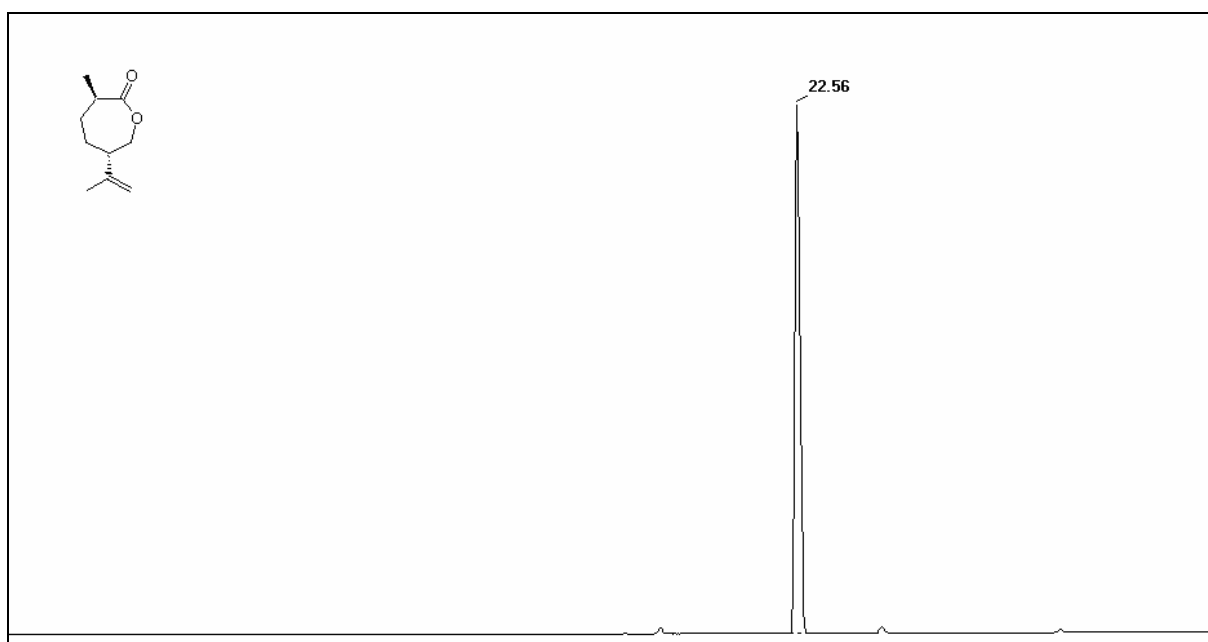
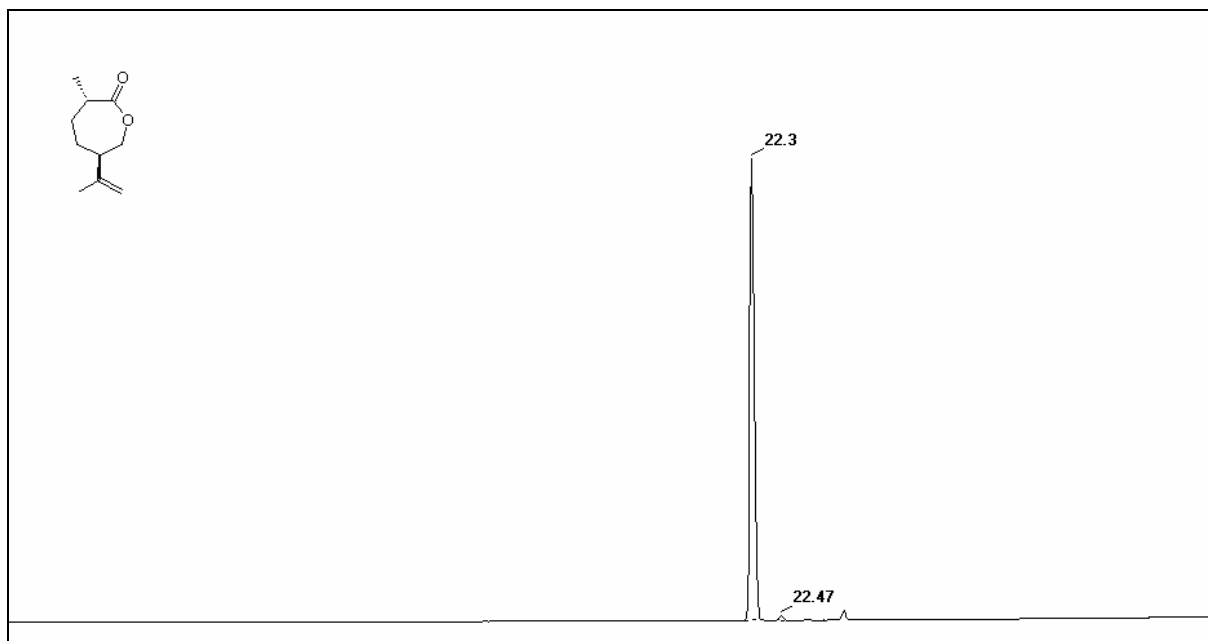
$^1\text{H}$  NMR of the "normal lactone" *trans*-7-Methyl-4-isopropenyl-2-oxo-oxepanone



<sup>13</sup>C NMR of the “normal lactone” *trans*-7-Methyl-4-isopropenyl-2-oxo-oxepanone



GC of the "abnormal lactone" *trans*-3-Methyl-6-isopropenyl-2-oxo-oxepanone



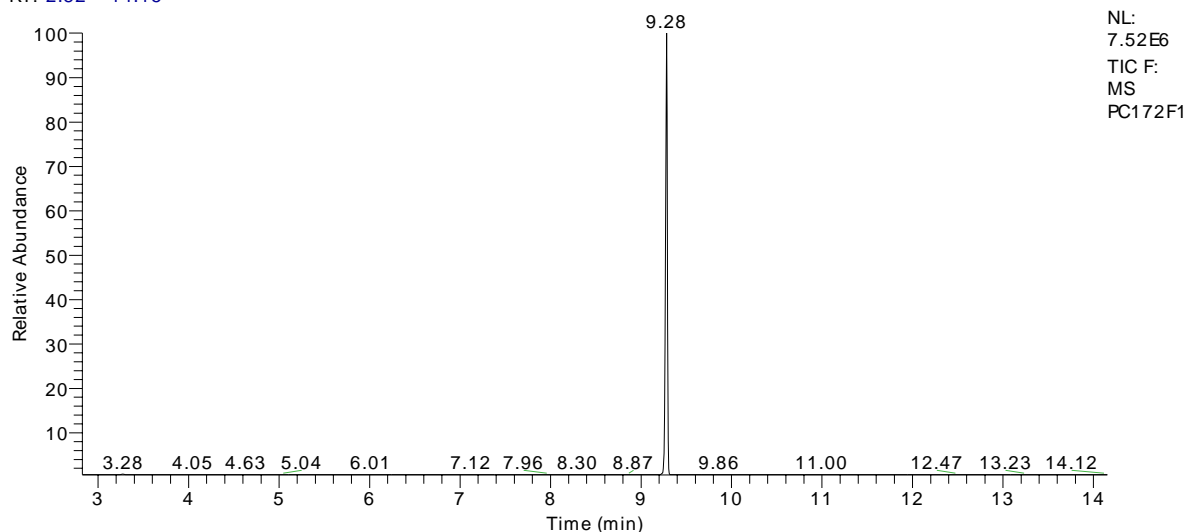
# GC MS of the "abnormal lactone" *trans*-3-Methyl-6-isopropenyl-2-oxo-oxepanone

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12. 9. 2006 20:21:25

PC172F1

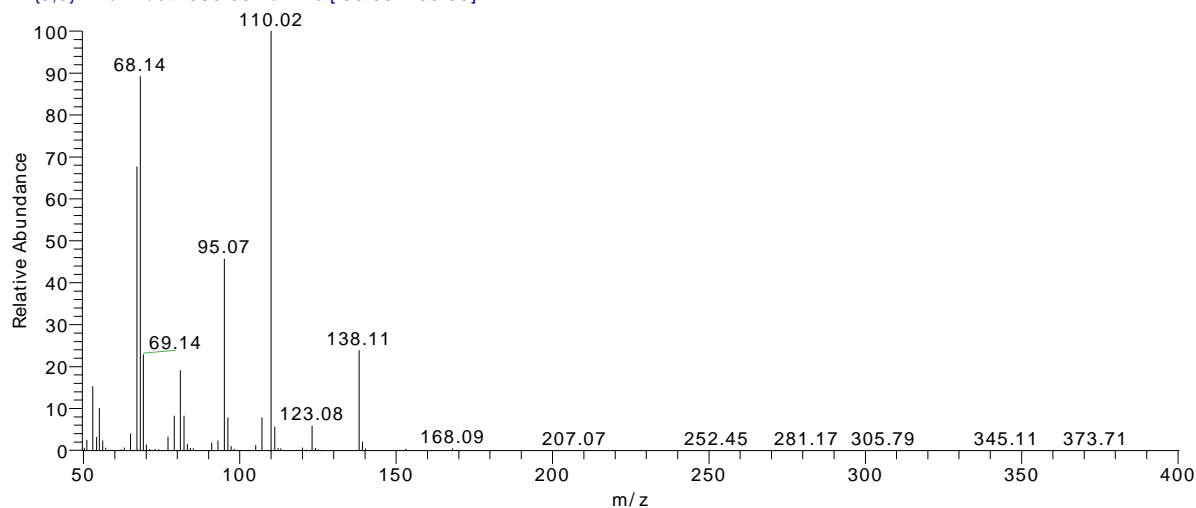
RT: 2.82 - 14.15



NL:  
7.52E6  
TIC F:  
MS  
PC172F1

PC172F1 #1310-1314 RT: 9.27-9.29 AV: 5 NL: 1.12E6

T: {0;0} + c EI det=350.00 Full ms [ 50.00-400.00]



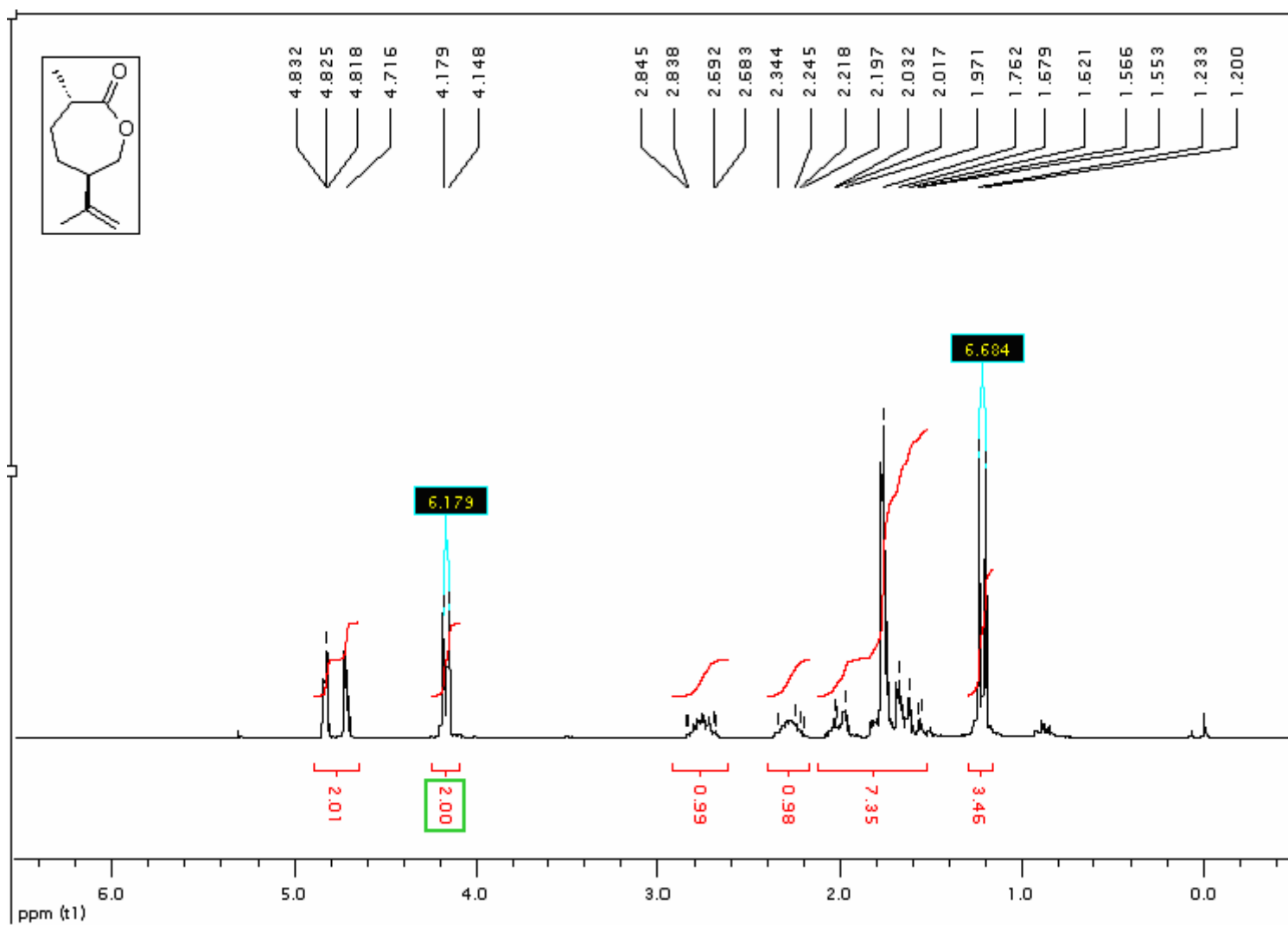
PC172F1#1310-1314 RT: 9.27-9.29 AV: 5

T: {0;0} + c EI det=350.00 Full ms [ 50.00-400.00]

m/z= 49.60-400.40

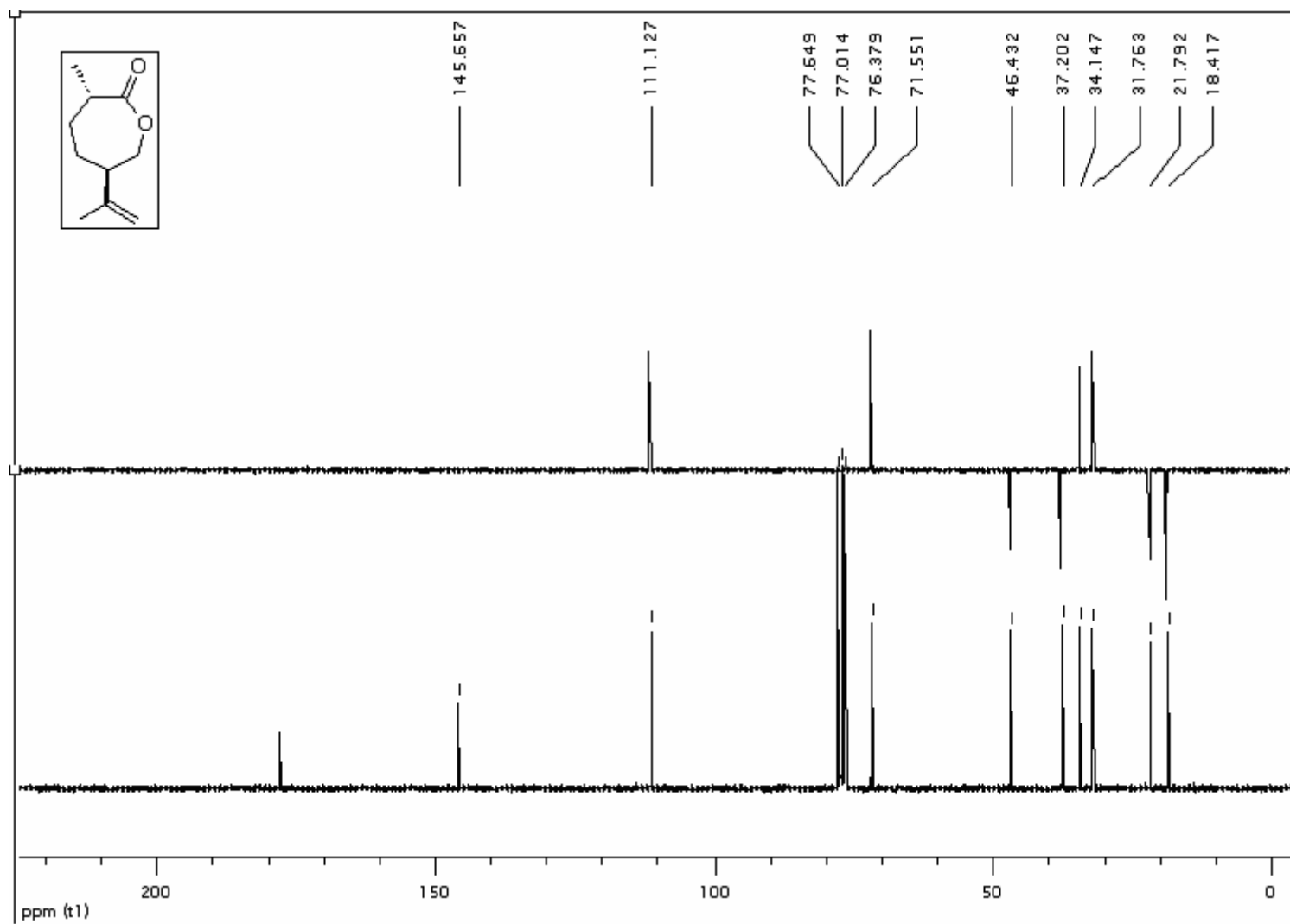
| m/z    | Intensity | Relative |
|--------|-----------|----------|
| 51.08  | 28096.0   | 2.51     |
| 52.97  | 171308.8  | 15.29    |
| 54.15  | 35447.2   | 3.16     |
| 55.11  | 113078.4  | 10.09    |
| 65.02  | 44672.0   | 3.99     |
| 67.07  | 758131.2  | 67.65    |
| 68.14  | 999424.0  | 89.18    |
| 69.14  | 256230.4  | 22.86    |
| 77.02  | 36312.8   | 3.24     |
| 78.99  | 92233.6   | 8.23     |
| 80.99  | 213408.0  | 19.04    |
| 82.15  | 92108.8   | 8.22     |
| 92.95  | 25740.8   | 2.30     |
| 95.07  | 512230.4  | 45.71    |
| 96.16  | 87715.2   | 7.83     |
| 107.06 | 87481.6   | 7.81     |

<sup>1</sup>H NMR of the “abnormal lactone” *trans*-3-Methyl-6-isopropenyl-2-oxo-oxepanone

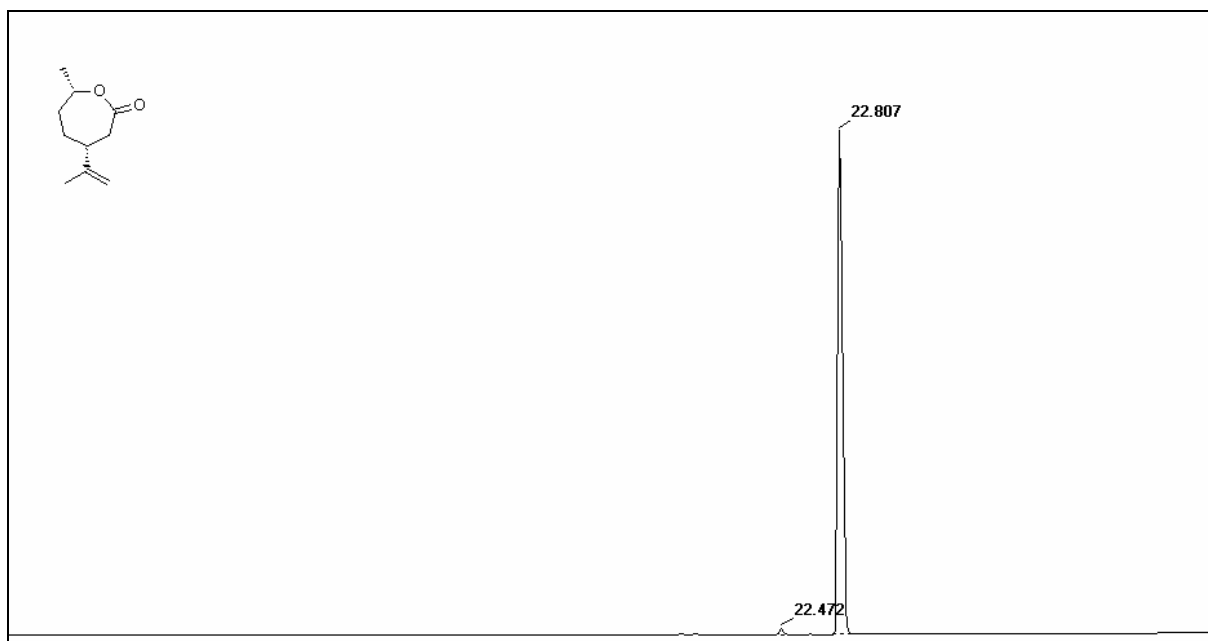
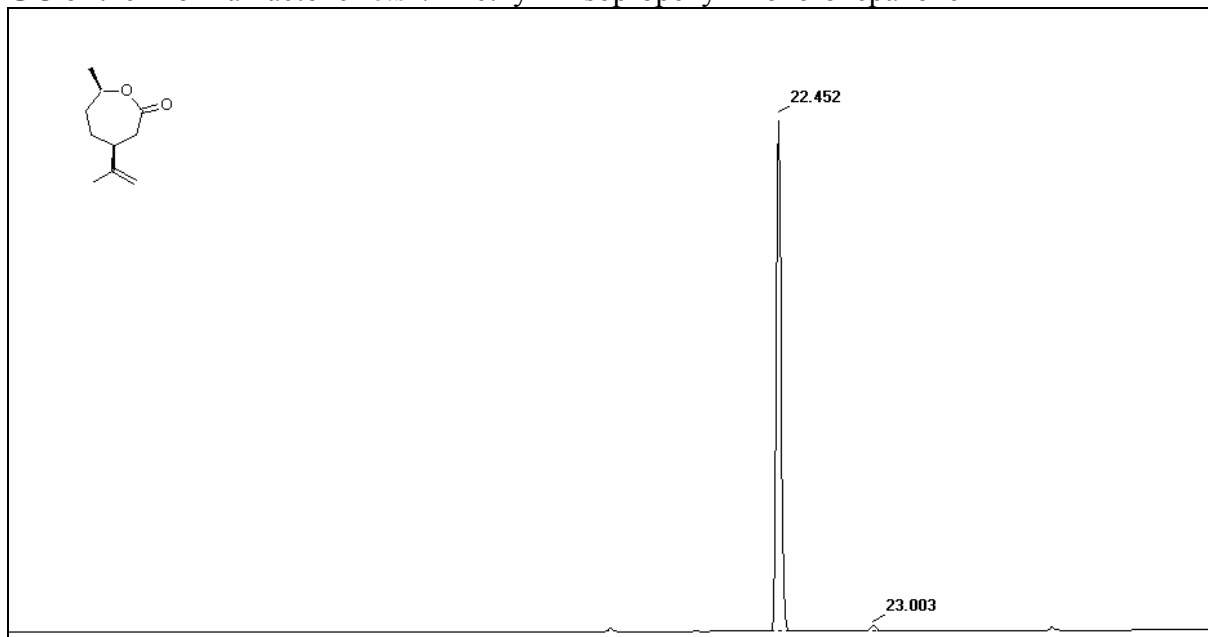




<sup>13</sup>C NMR of the “abnormal lactone” *trans*-3-Methyl-6-isopropenyl-2-oxo-oxepanone



GC of the "normal lactone" *cis*-7-Methyl-4-isopropenyl-2-oxo-oxepanone



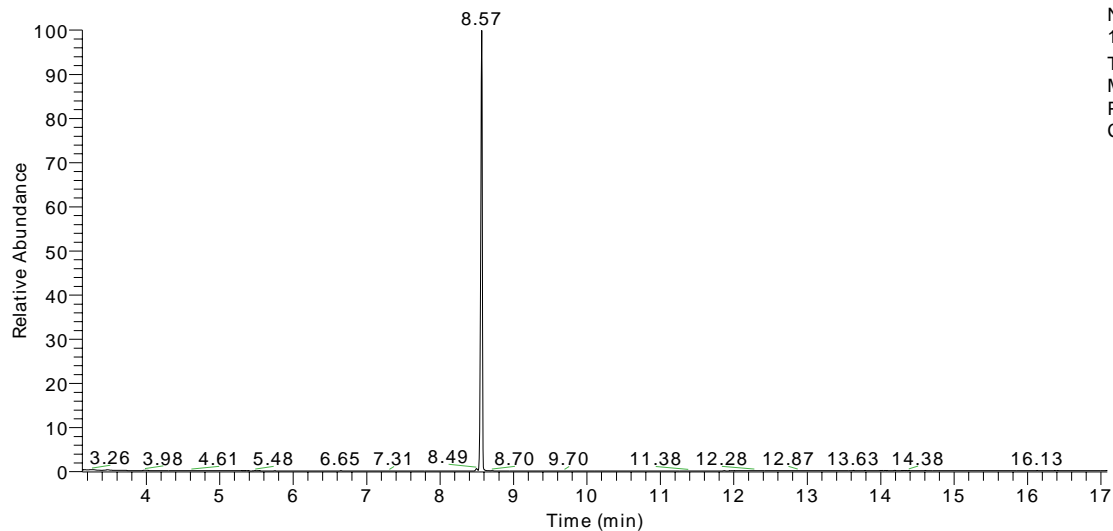
# GC of the "normal lactone" *cis*-7-Methyl-4-isopropenyl-2-oxo-oxepanone

D:\Dokumenty\vi eden\GCMS.PC213-CHMO-F1

7. 9. 2006 18:07:29

PC213-CHMO-F1

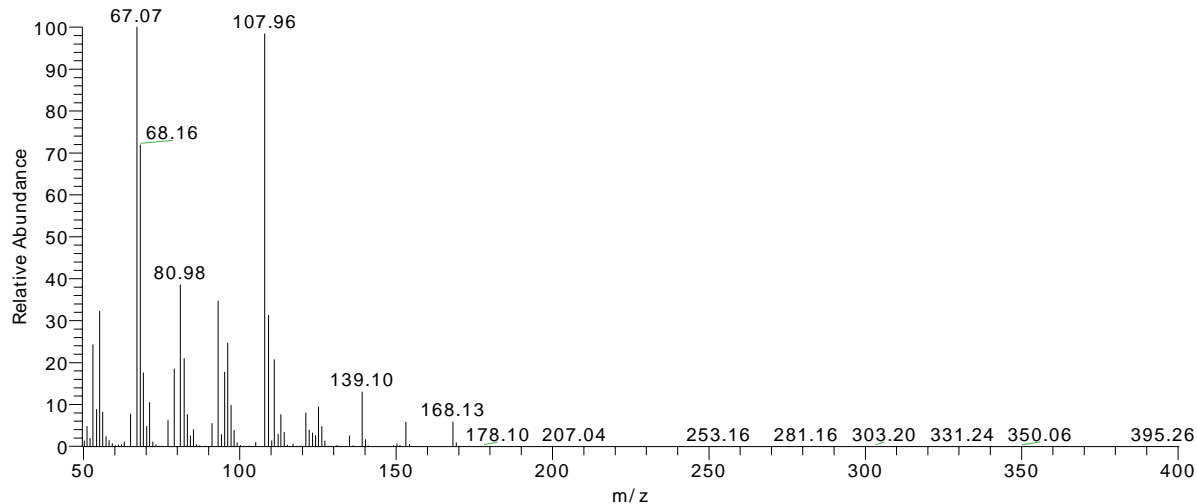
RT: 3.13 - 17.08



NL:  
1.11E7  
TIC F:  
MS  
PC213-  
CHMO-F1

PC213-CHMO-F1 #951-956 RT: 8.55-8.58 AV: 6 NL: 1.04E6

T: {0;0} + c EI det=350.00 Full ms [ 50.00-400.00]



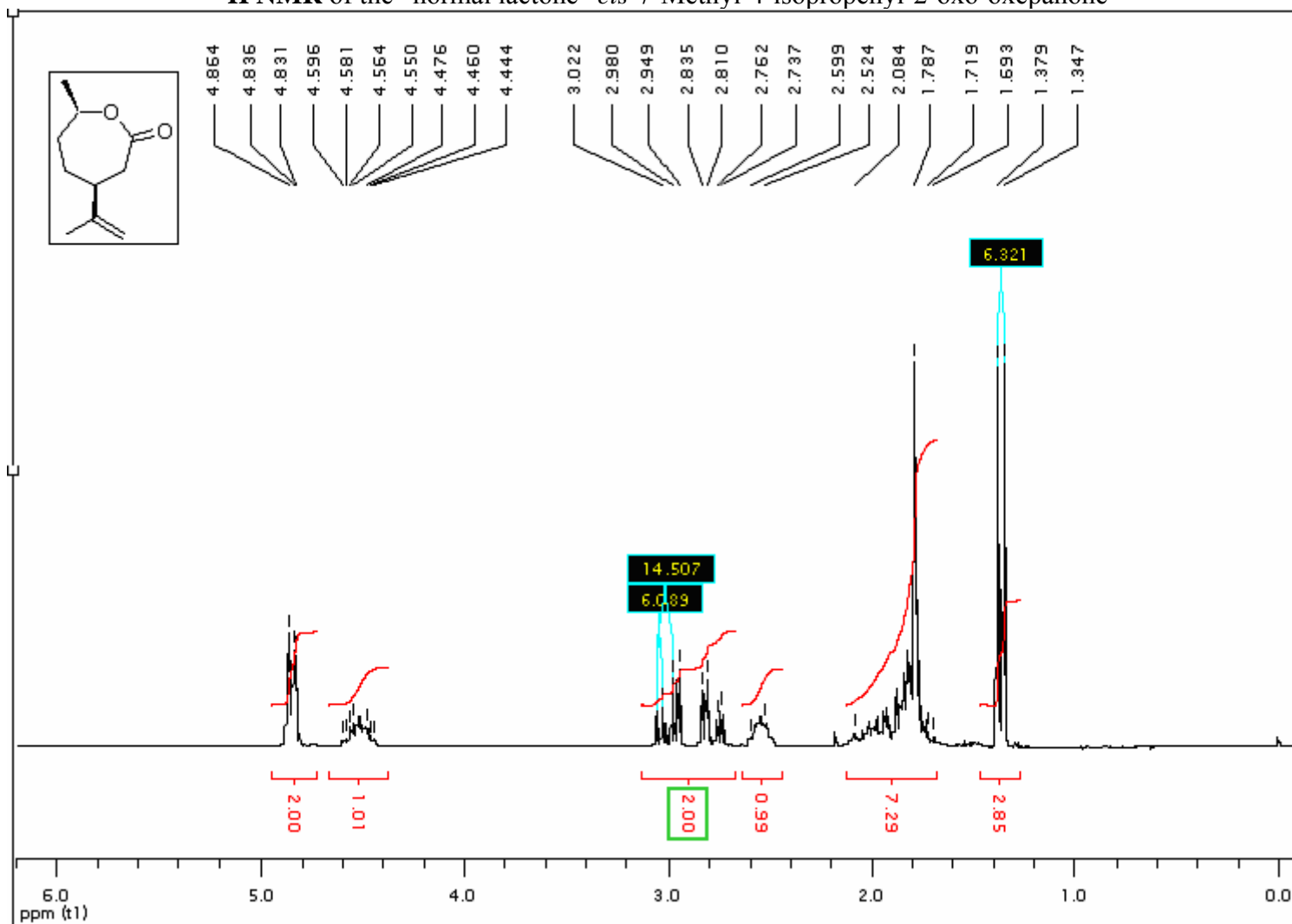
PC213-CHMO-F1#951-956 RT: 8.55-8.58 AV: 6

T: {0;0} + c EI det=350.00 Full ms [ 50.00-400.00]

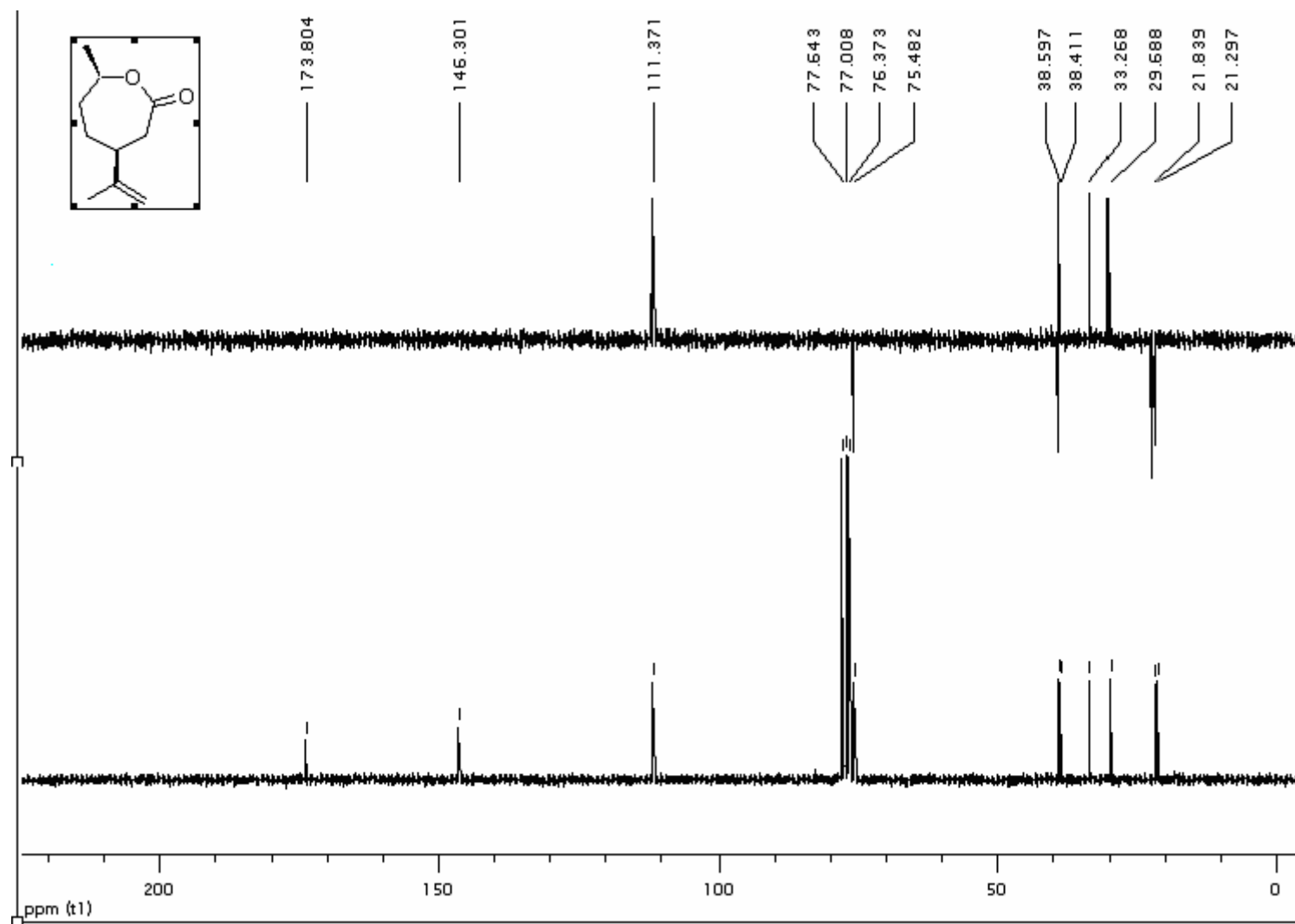
m/z= 49.60-400.40

| m/z    | Intensity | Relative |
|--------|-----------|----------|
| 53.03  | 253058.7  | 24.25    |
| 54.17  | 92005.3   | 8.82     |
| 55.13  | 336821.3  | 32.28    |
| 56.17  | 85144.0   | 8.16     |
| 67.07  | 1043413.3 | 100.00   |
| 68.16  | 750624.0  | 71.94    |
| 69.17  | 183578.7  | 17.59    |
| 71.12  | 109653.3  | 10.51    |
| 79.03  | 193405.3  | 18.54    |
| 80.98  | 402421.3  | 38.57    |
| 82.17  | 218981.3  | 20.99    |
| 93.07  | 361813.3  | 34.68    |
| 95.09  | 185112.0  | 17.74    |
| 96.14  | 257794.7  | 24.71    |
| 97.16  | 102413.3  | 9.82     |
| 107.96 | 1026965.3 | 98.42    |

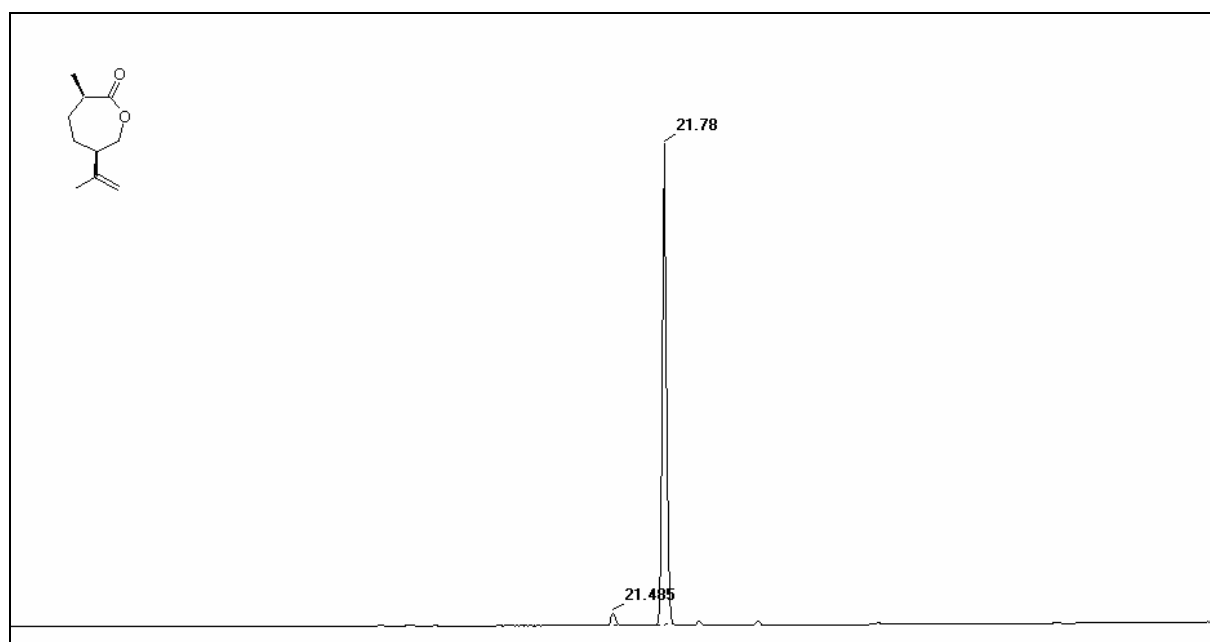
<sup>1</sup>H NMR of the "normal lactone" *cis*-7-Methyl-4-isopropenyl-2-oxo-oxepanone



<sup>13</sup>C NMR of the “normal lactone” *cis*-7-Methyl-4-isopropenyl-2-oxo-oxepanone



GC of the "abnormal lactone" *cis*-3-Methyl-6-isopropenyl-2-oxo-oxepanone



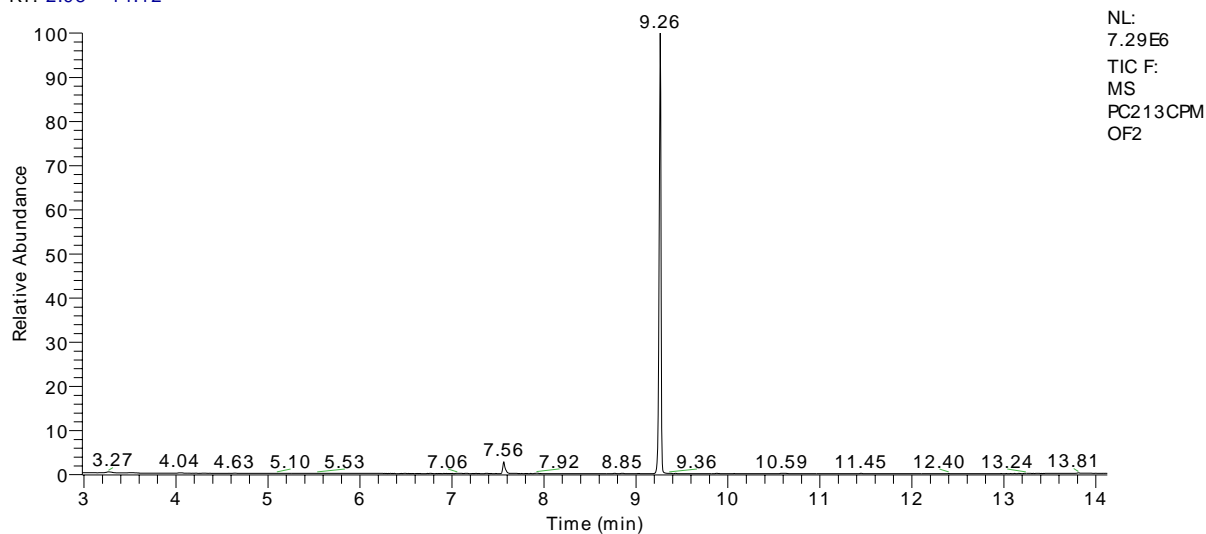
# GC MS of the "abnormal lactone" *cis*-3-Methyl-6-isopropenyl-2-oxo-oxepanone

D:\Dokumenty\viaden\GCMS.PC213CPMOF2

12. 9. 2006 21:42:06

PC213CPMOF2

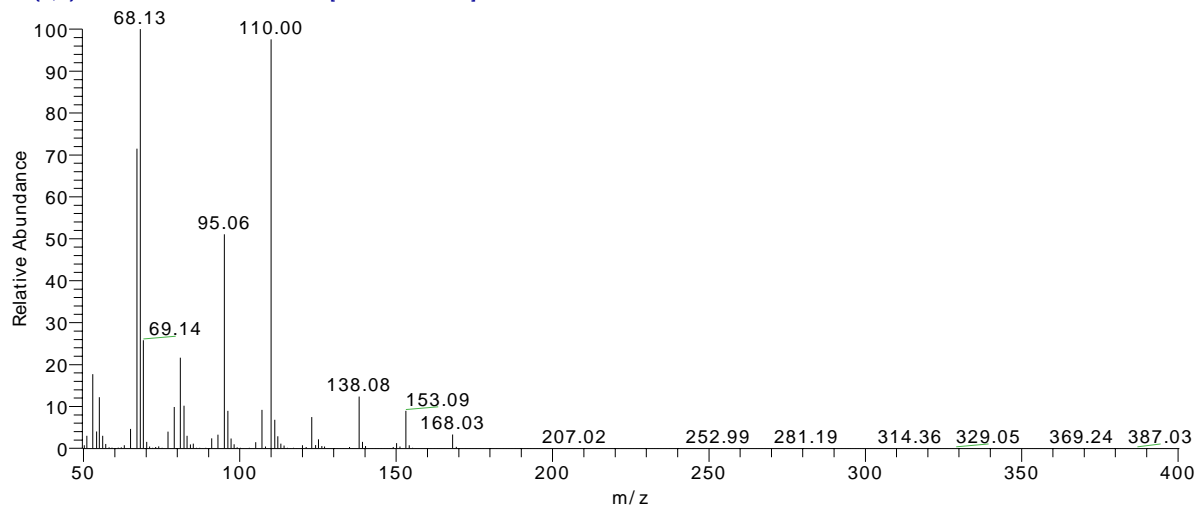
RT: 2.98 - 14.12



NL:  
7.29E6  
TIC F:  
MS  
PC213CPM  
OF2

PC213CPMOF2 #1307-1311 RT: 9.25-9.28 AV: 5 NL: 9.85E5

T: {0;0} + c EI det=350.00 Full ms [ 50.00-400.00]



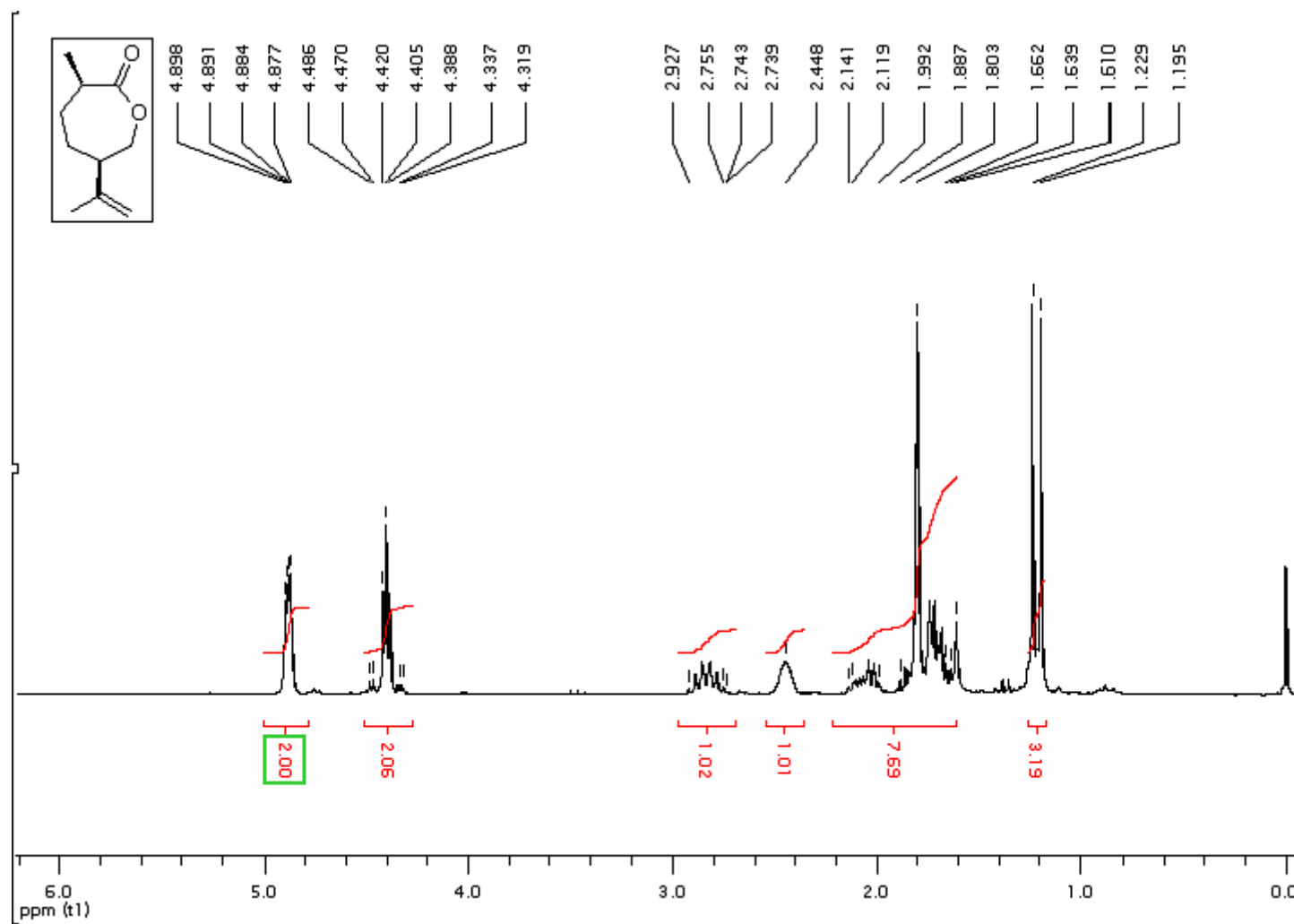
PC213CPMOF2#1307-1311 RT: 9.25-9.28 AV: 5

T: {0;0} + c EI det=350.00 Full ms [ 50.00-400.00]

m/z= 49.60-400.40

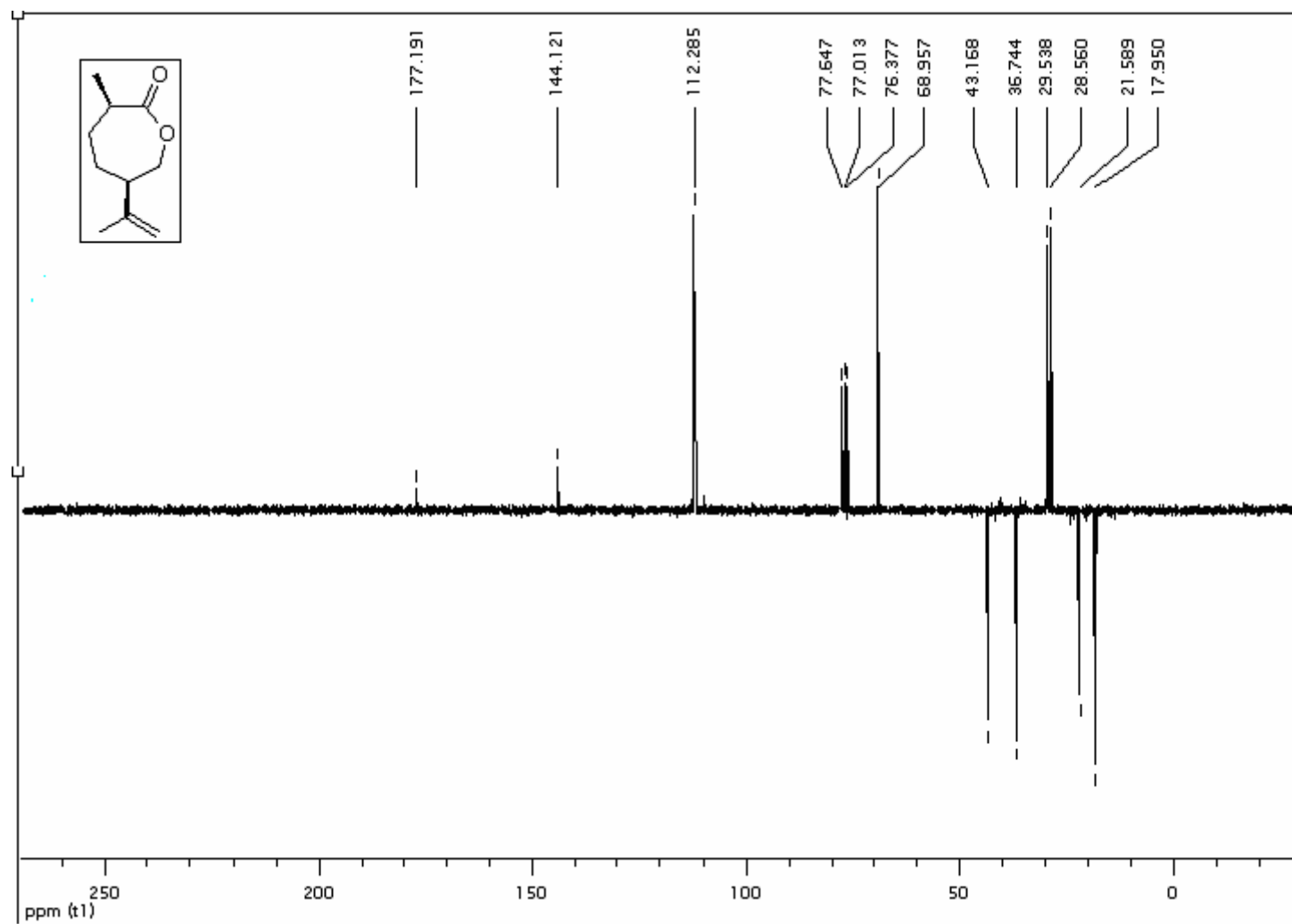
| m/z    | Intensity | Relative |
|--------|-----------|----------|
| 52.96  | 173664.0  | 17.63    |
| 54.15  | 39457.6   | 4.01     |
| 55.11  | 119920.0  | 12.18    |
| 65.02  | 45547.2   | 4.62     |
| 67.06  | 704038.4  | 71.48    |
| 68.13  | 984934.4  | 100.00   |
| 69.14  | 253196.8  | 25.71    |
| 77.02  | 38886.4   | 3.95     |
| 78.99  | 96867.2   | 9.83     |
| 80.99  | 212652.8  | 21.59    |
| 82.15  | 99548.8   | 10.11    |
| 95.06  | 502310.4  | 51.00    |
| 96.16  | 87420.8   | 8.88     |
| 107.06 | 89859.2   | 9.12     |
| 110.00 | 960588.8  | 97.53    |
| 111.17 | 66707.2   | 6.77     |

<sup>1</sup>H NMR of the “abnormal lactone” *cis*-3-Methyl-6-isopropenyl-2-oxo-oxepanone

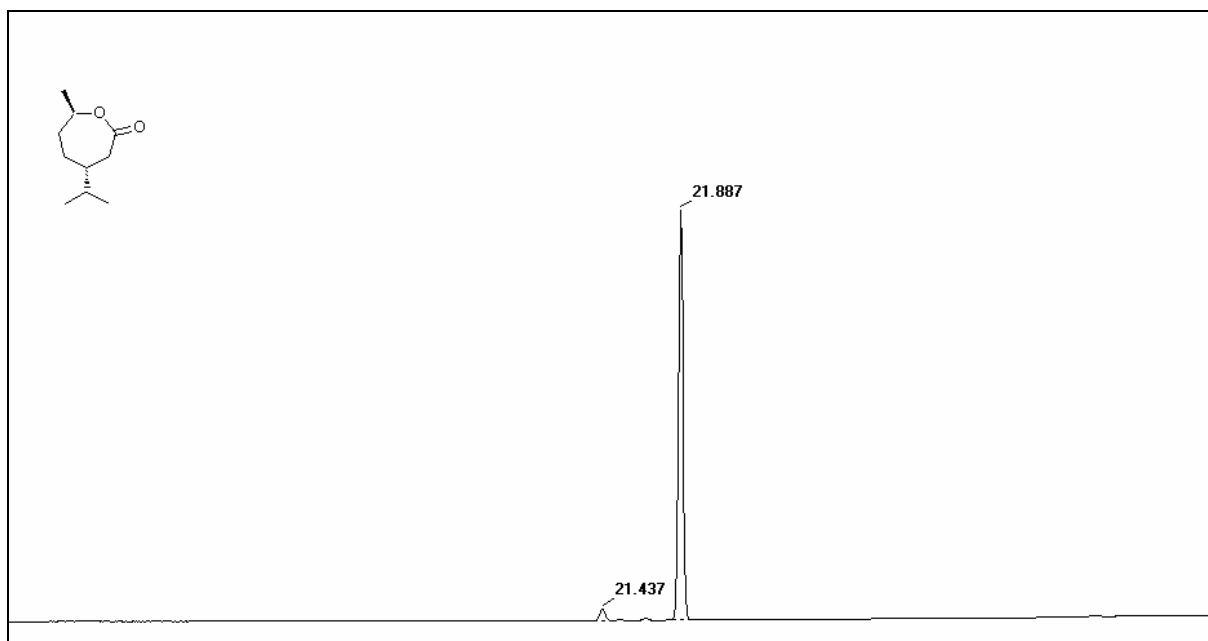
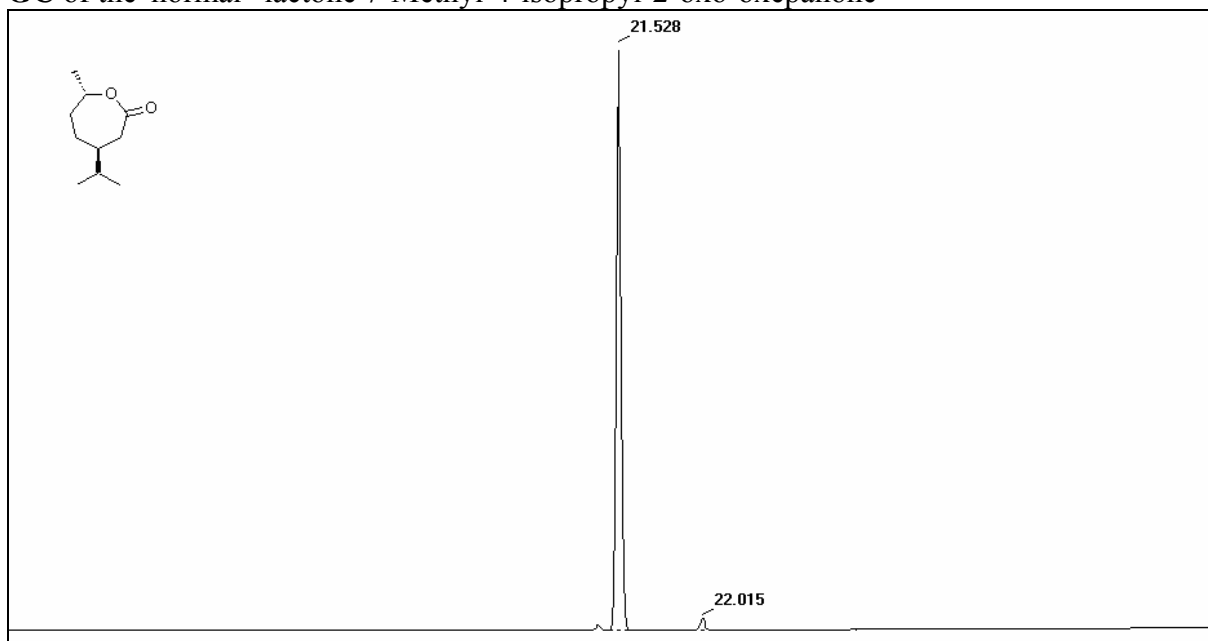




<sup>13</sup>C NMR of the “abnormal lactone” *cis*-3-Methyl-6-isopropenyl-2-oxo-oxepanone



GC of the "normal" lactone 7-Methyl-4-isopropyl-2-oxo-oxepanone



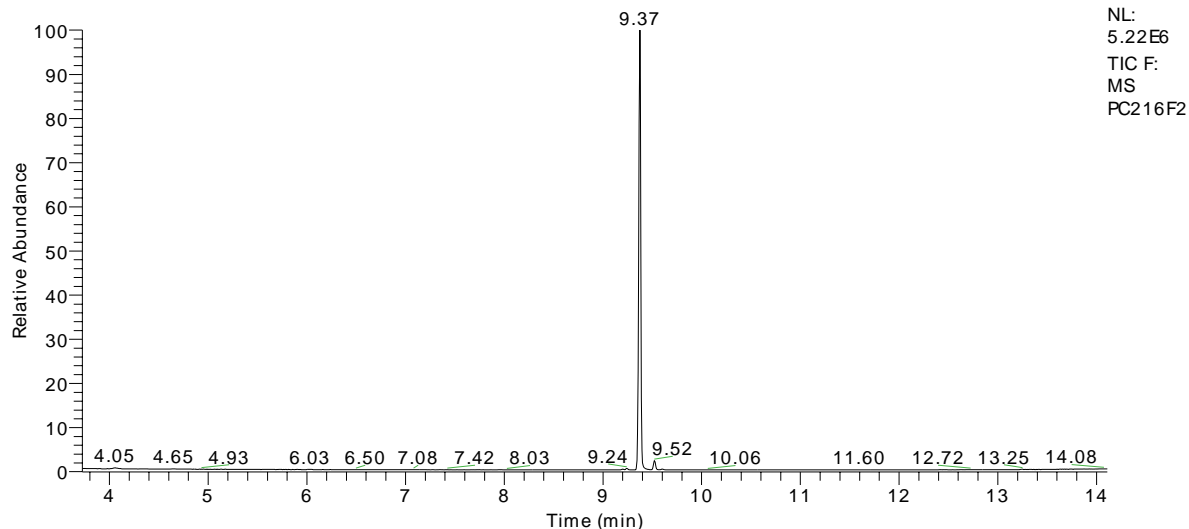
# GC MS of the „normal“ lactone 7-Methyl-4-isopropyl-2-oxo-oxepanone

D:\Dokumenty\viaden\GCMS.PC216F2

26. 9. 2006 14:28:13

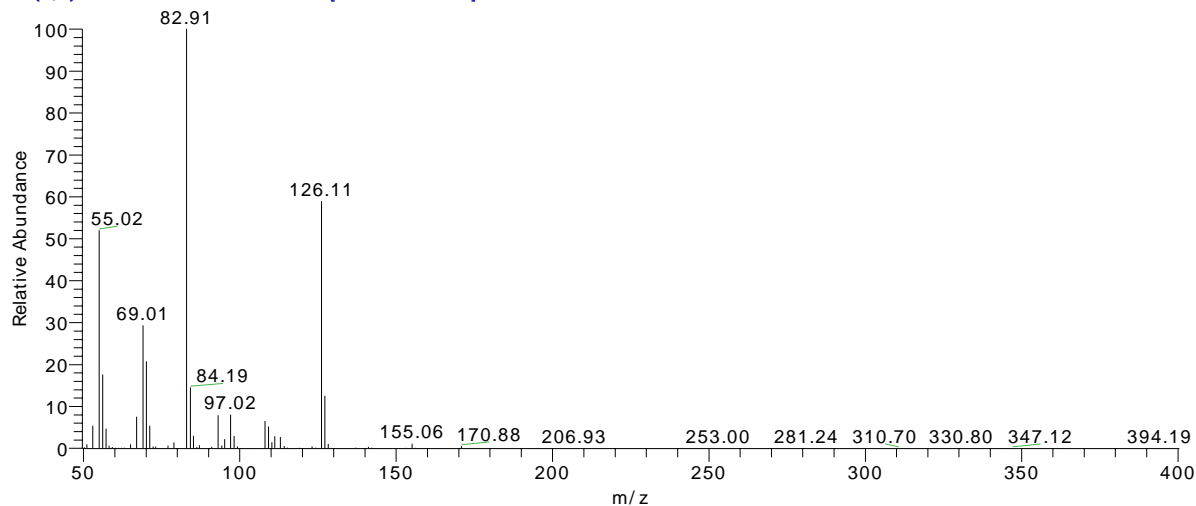
PC216F2

RT: 3.72 - 14.11



NL:  
5.22E6  
TIC F:  
MS  
PC216F2

PC216F2 #1328 RT: 9.37 AV: 1 NL: 1.35E6  
T: {0;0} + c EI det=350.00 Full ms [ 50.00-400.00]



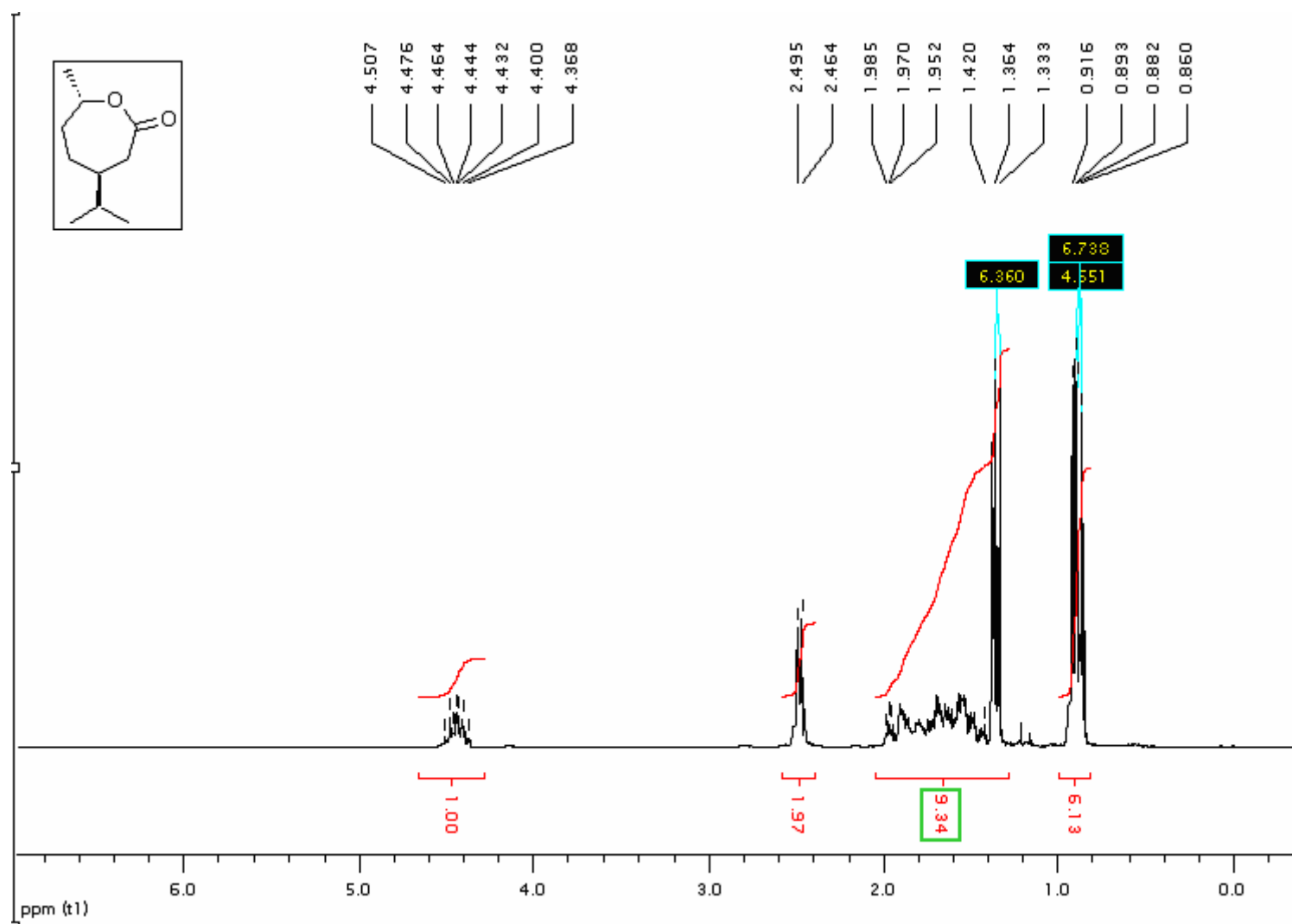
PC216F2#1328 RT: 9.37

T: {0;0} + c EI det=350.00 Full ms [ 50.00-400.00]

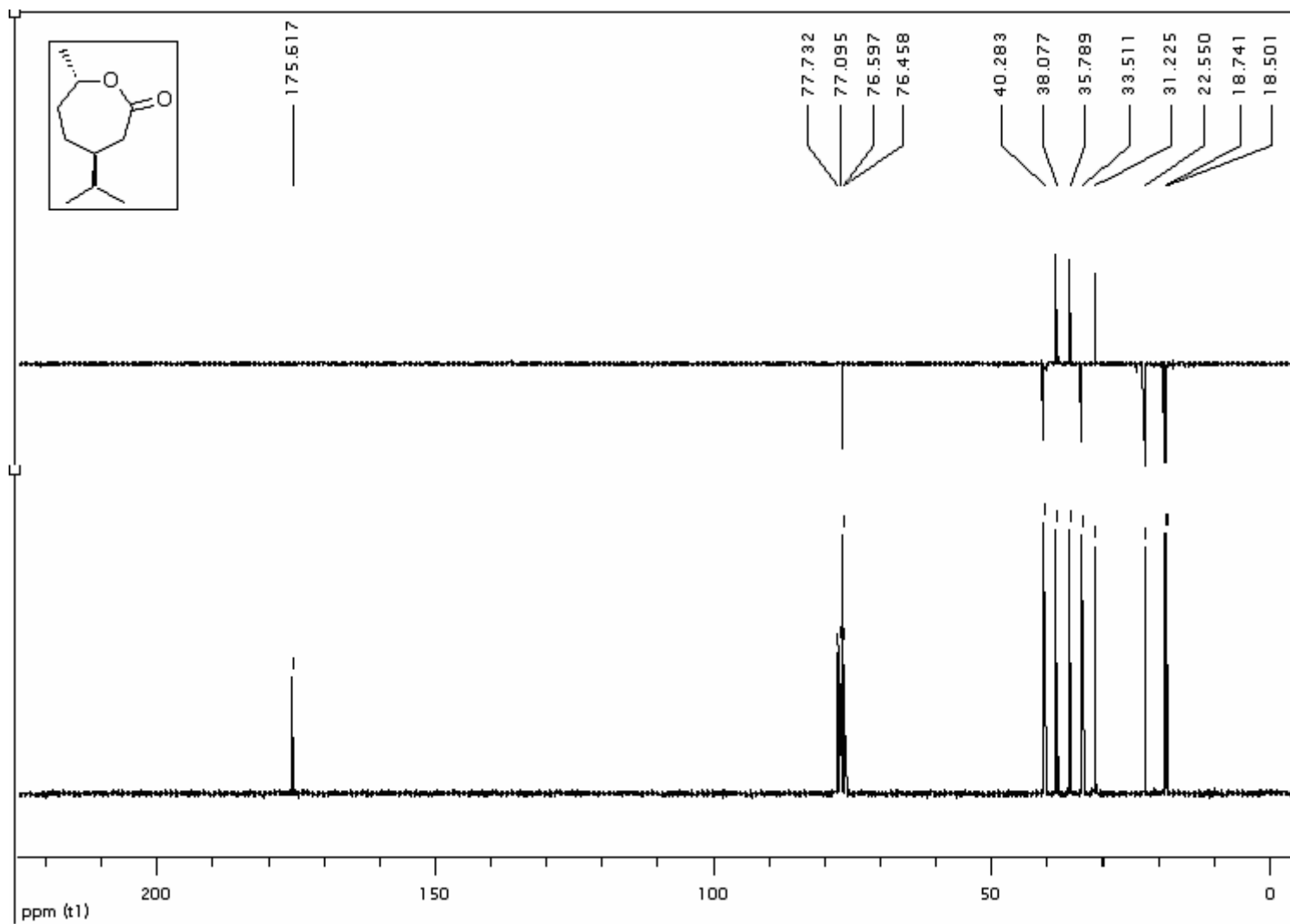
m/z= 49.60-400.40

| m/z    | Intensity | Relative |
|--------|-----------|----------|
| 52.96  | 72352.0   | 5.35     |
| 55.02  | 702464.0  | 51.99    |
| 56.17  | 238080.0  | 17.62    |
| 57.17  | 63472.0   | 4.70     |
| 66.99  | 101680.0  | 7.53     |
| 69.01  | 395264.0  | 29.25    |
| 70.15  | 280064.0  | 20.73    |
| 71.16  | 72480.0   | 5.36     |
| 82.91  | 1351168.0 | 100.00   |
| 84.19  | 195968.0  | 14.50    |
| 85.18  | 39984.0   | 2.96     |
| 93.02  | 106144.0  | 7.86     |
| 97.02  | 107824.0  | 7.98     |
| 98.15  | 39392.0   | 2.92     |
| 108.06 | 87632.0   | 6.49     |
| 109.17 | 70176.0   | 5.19     |

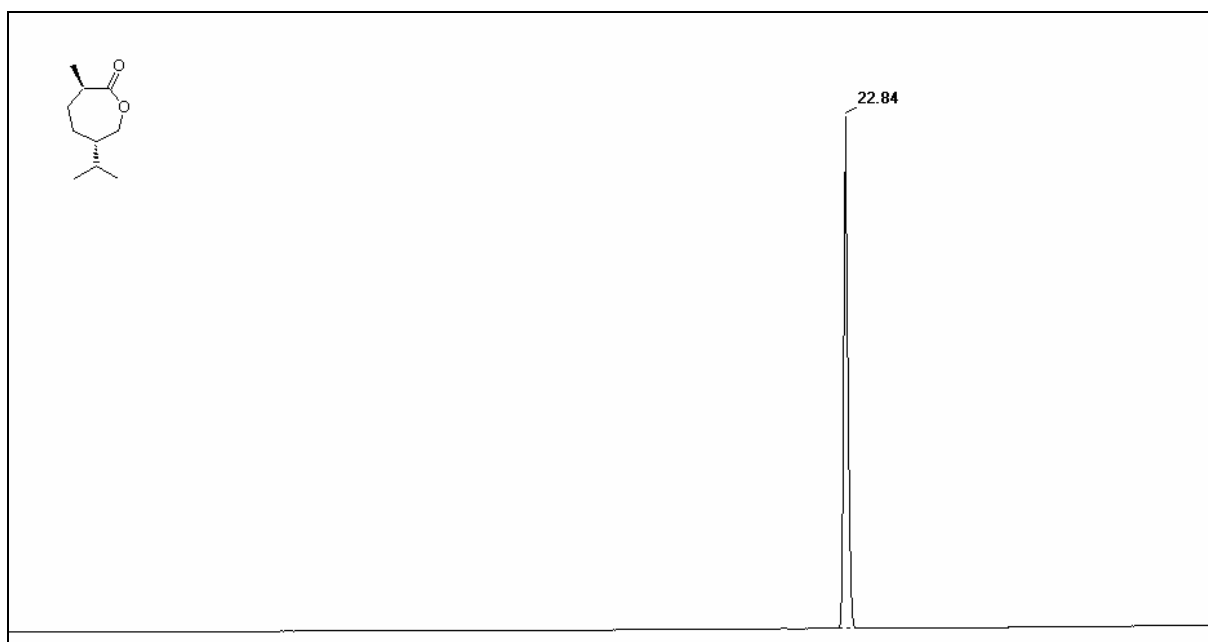
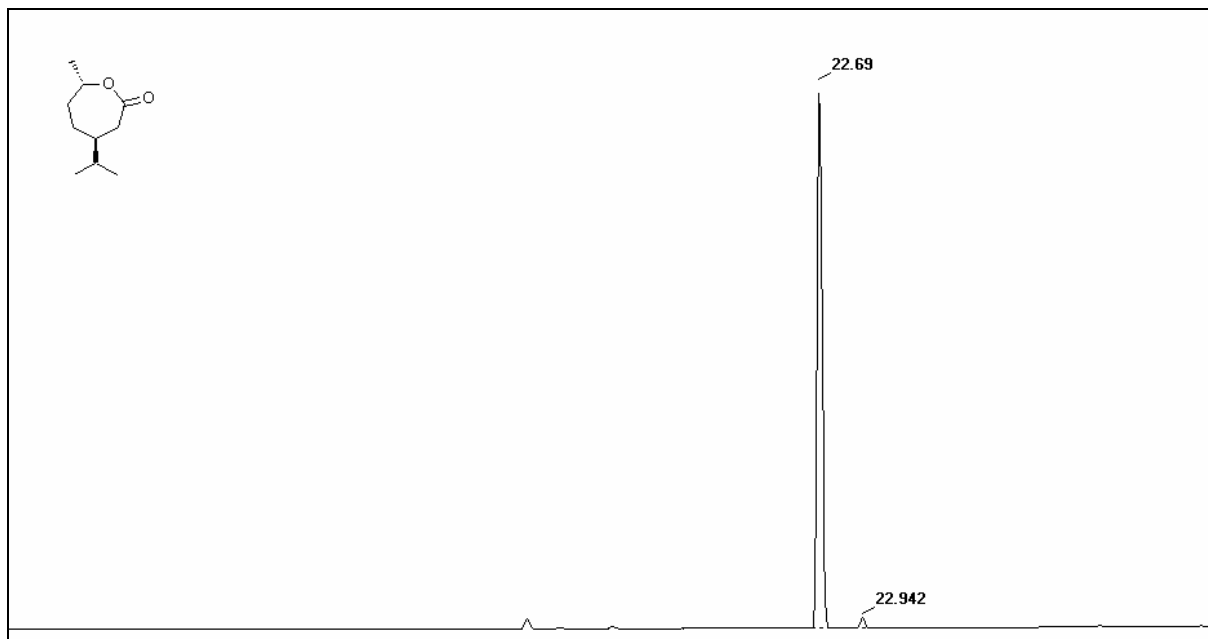
<sup>1</sup>H NMR of the „normal“ lactone 7-Methyl-4-isopropyl-2-oxo-oxepanone



<sup>13</sup>C NMR of the „normal“ lactone 7-Methyl-4-isopropyl-2-oxo-oxepanone



GC of the „abnormal“ lactone of 3-Methyl-6-isopropyl-2-oxo-oxepanone



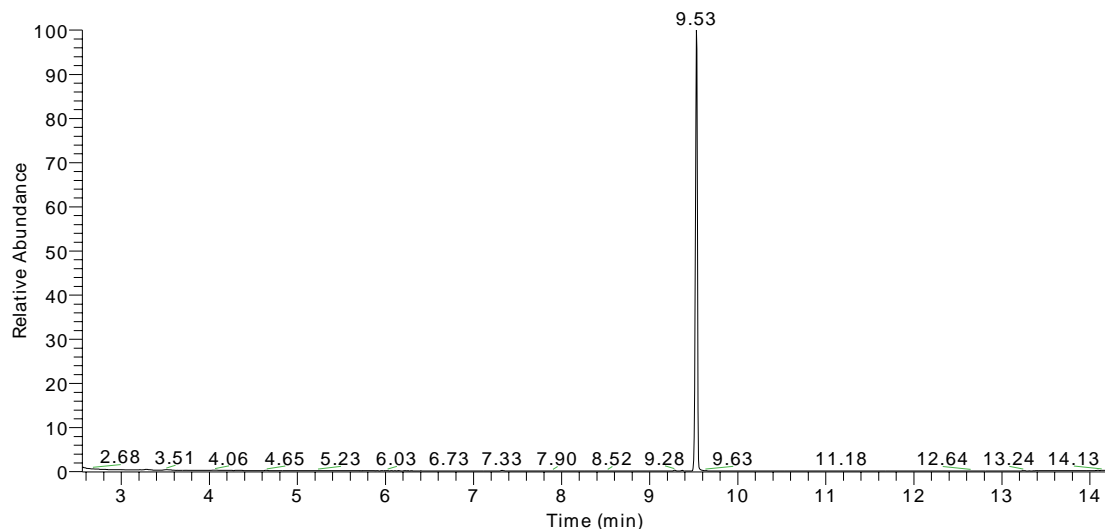
# GC MS of the „abnormal“ lactone of 3-Methyl-6-isopropyl-2-oxo-oxepanone

D:\Dokumenty\viaden\GCMS.PC216F1

26. 9. 2006 14:07:44

PC216F1

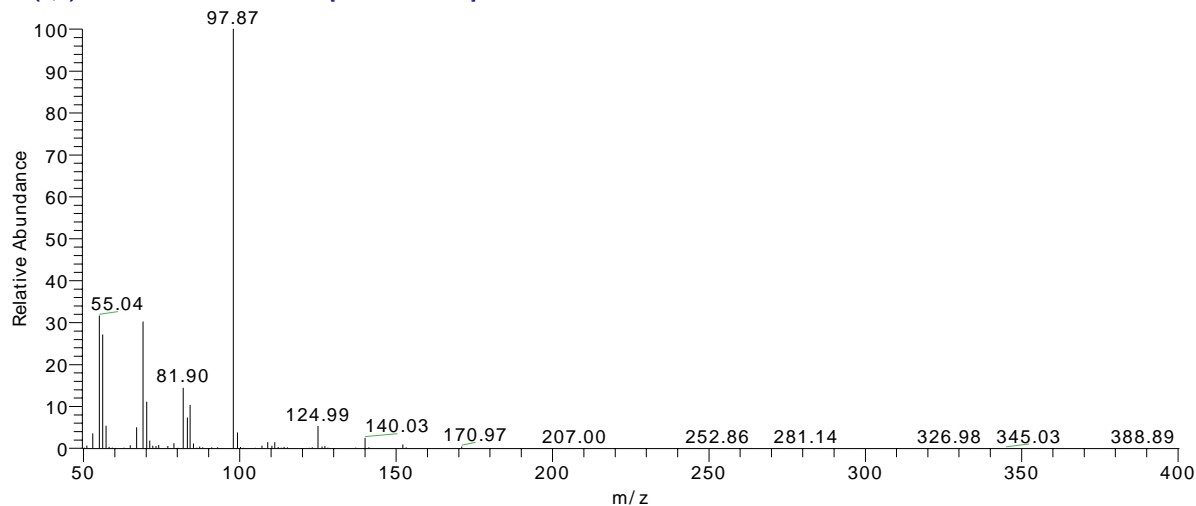
RT: 2.56 - 14.20



NL:  
1.08E7  
TIC F:  
MS  
PC216F1

PC216F1 #1353-1358 RT: 9.51-9.54 AV: 6 NL: 2.74E6

T: {0;0} + c EI det=350.00 Full ms [ 50.00-400.00]



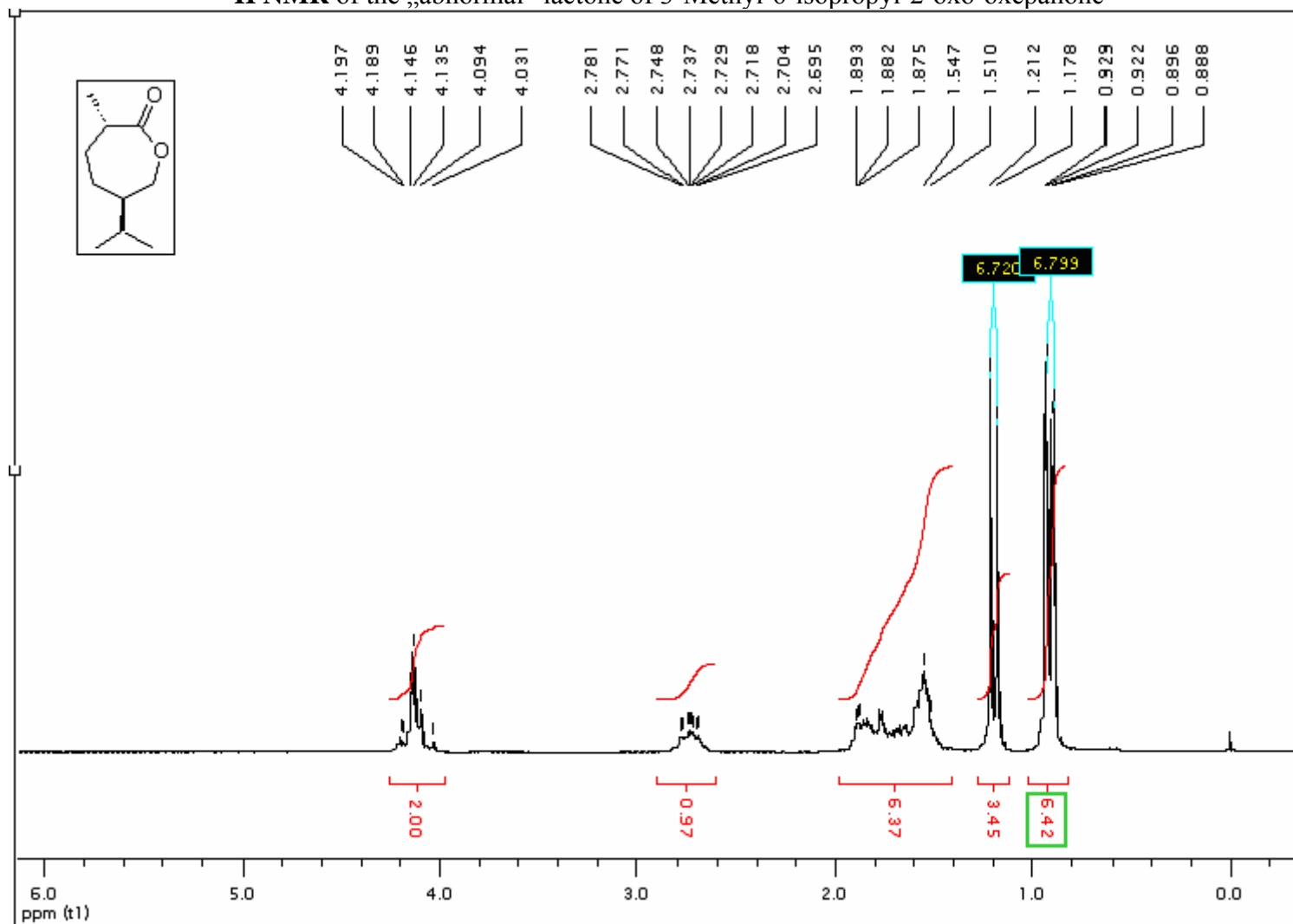
PC216F1#1353-1358 RT: 9.51-9.54 AV: 6

T: {0;0} + c EI det=350.00 Full ms [ 50.00-400.00]

m/z= 49.60-400.40

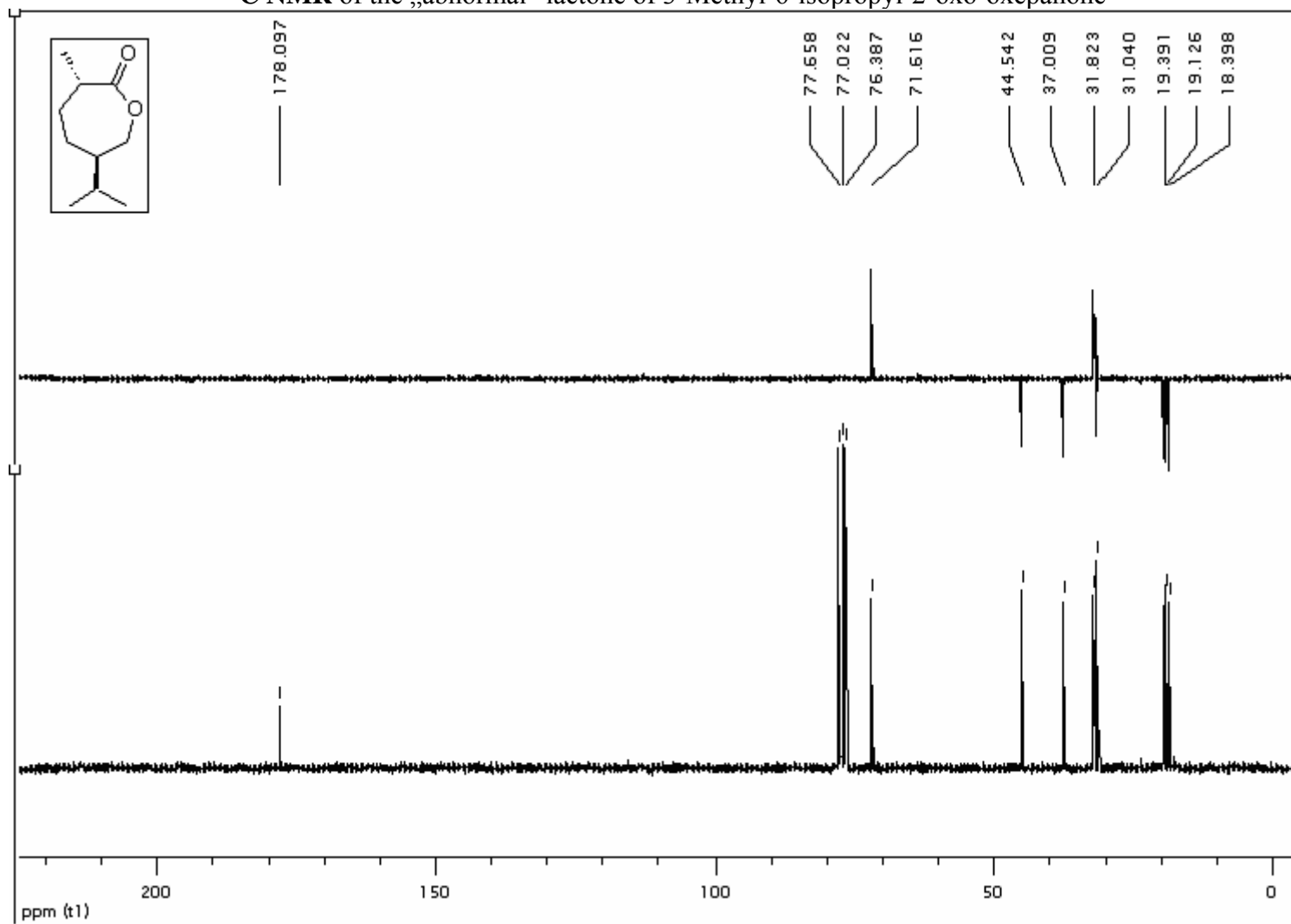
| m/z    | Intensity | Relative |
|--------|-----------|----------|
| 52.95  | 96501.3   | 3.52     |
| 55.04  | 868128.0  | 31.64    |
| 56.15  | 744256.0  | 27.12    |
| 57.17  | 147469.3  | 5.37     |
| 67.00  | 136616.0  | 4.98     |
| 69.02  | 828341.3  | 30.19    |
| 70.16  | 305482.7  | 11.13    |
| 71.19  | 49136.0   | 1.79     |
| 78.96  | 32231.3   | 1.17     |
| 81.90  | 396042.7  | 14.43    |
| 83.19  | 199997.3  | 7.29     |
| 84.14  | 282421.3  | 10.29    |
| 85.19  | 30257.3   | 1.10     |
| 97.87  | 2743893.3 | 100.00   |
| 99.20  | 102589.3  | 3.74     |
| 108.97 | 39590.7   | 1.44     |

<sup>1</sup>H NMR of the „abnormal“ lactone of 3-Methyl-6-isopropyl-2-oxo-oxepanone

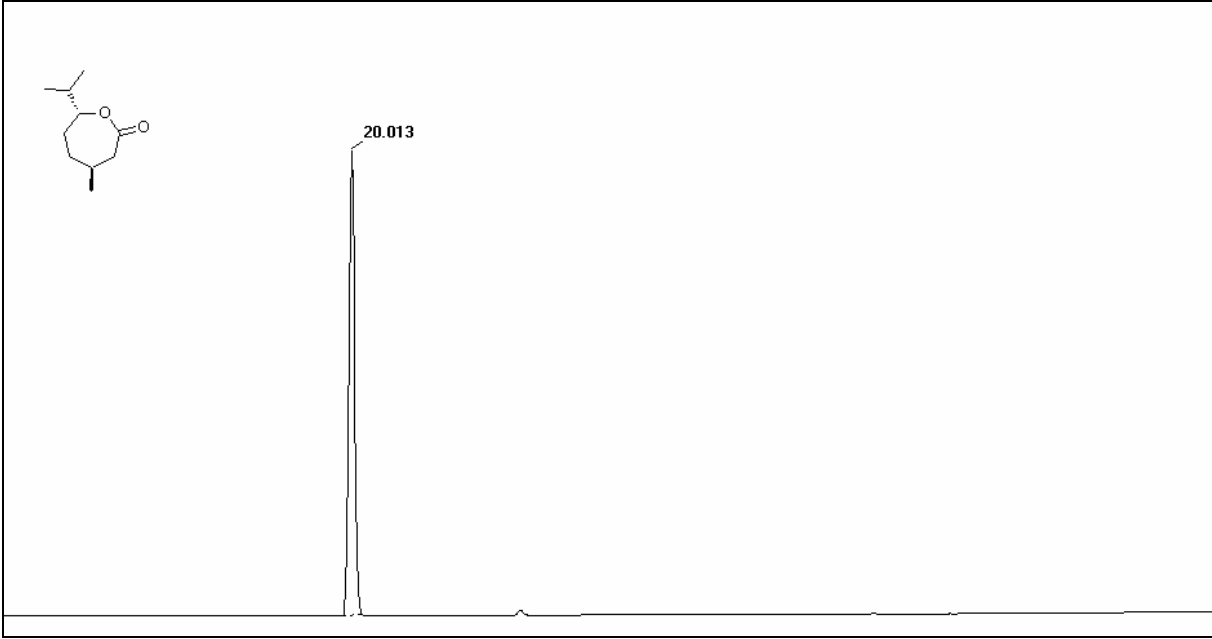




<sup>13</sup>C NMR of the „abnormal“ lactone of 3-Methyl-6-isopropyl-2-oxo-oxepanone



GC of the „normal“ lactone 4-Methyl-7-isopropyl-2-oxo-oxepanone



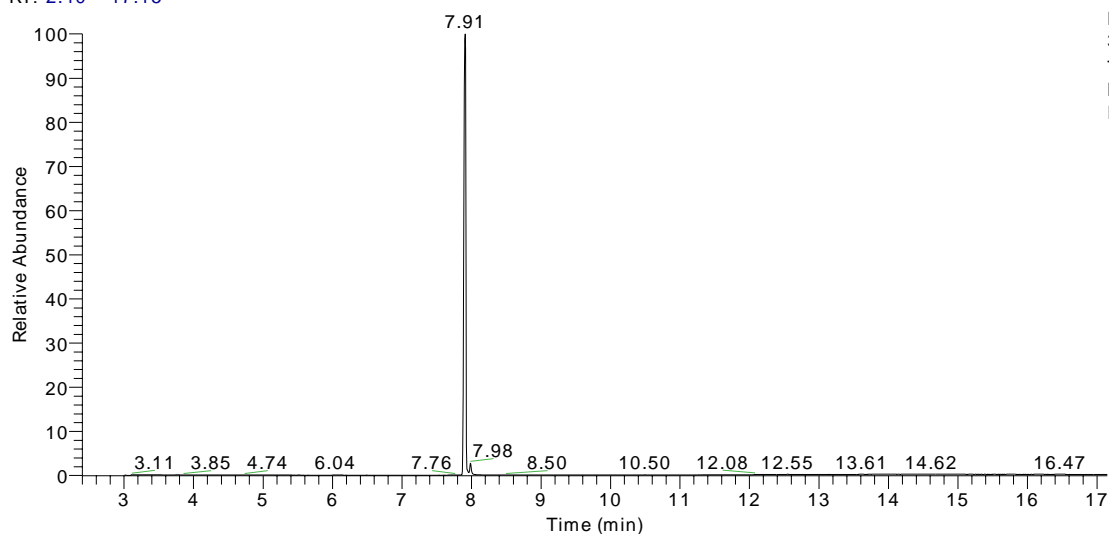
# GC MS of the „normal“ lactone 4-Methyl-7-isopropyl-2-oxo-oxepanone

D:\Dokumenty\...\februar2007\PC181-f1

6. 2. 2007 18:07:55

PC181-f1

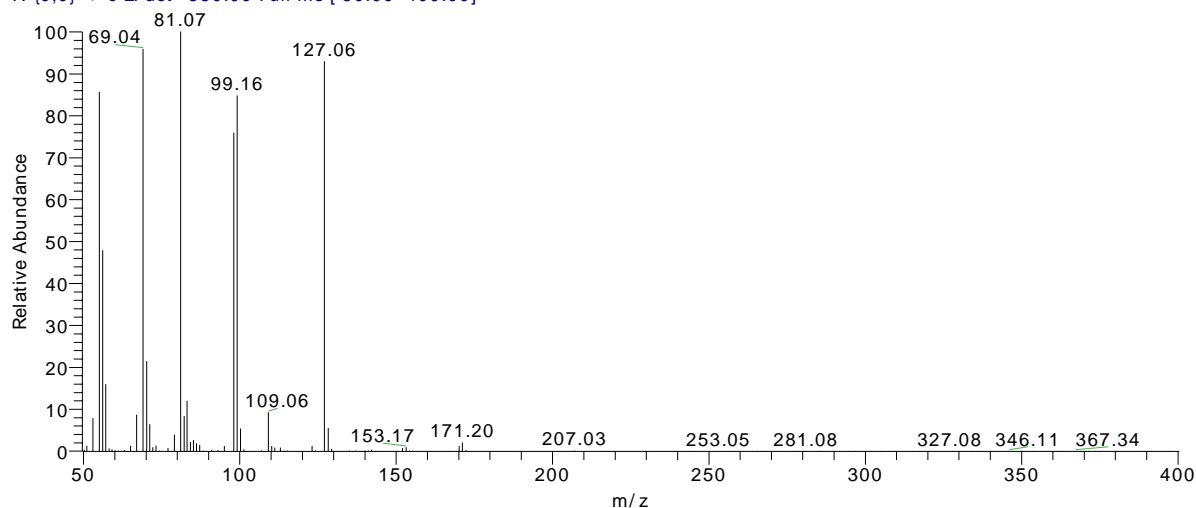
RT: 2.40 - 17.15



NL:  
3.47E7  
TIC F:  
MS  
PC181-f1

PC181-f1 #816-821 RT: 7.89-7.92 AV: 6 NL: 4.02E6

T: {0;0} + c EI det=350.00 Full ms [ 50.00-400.00]



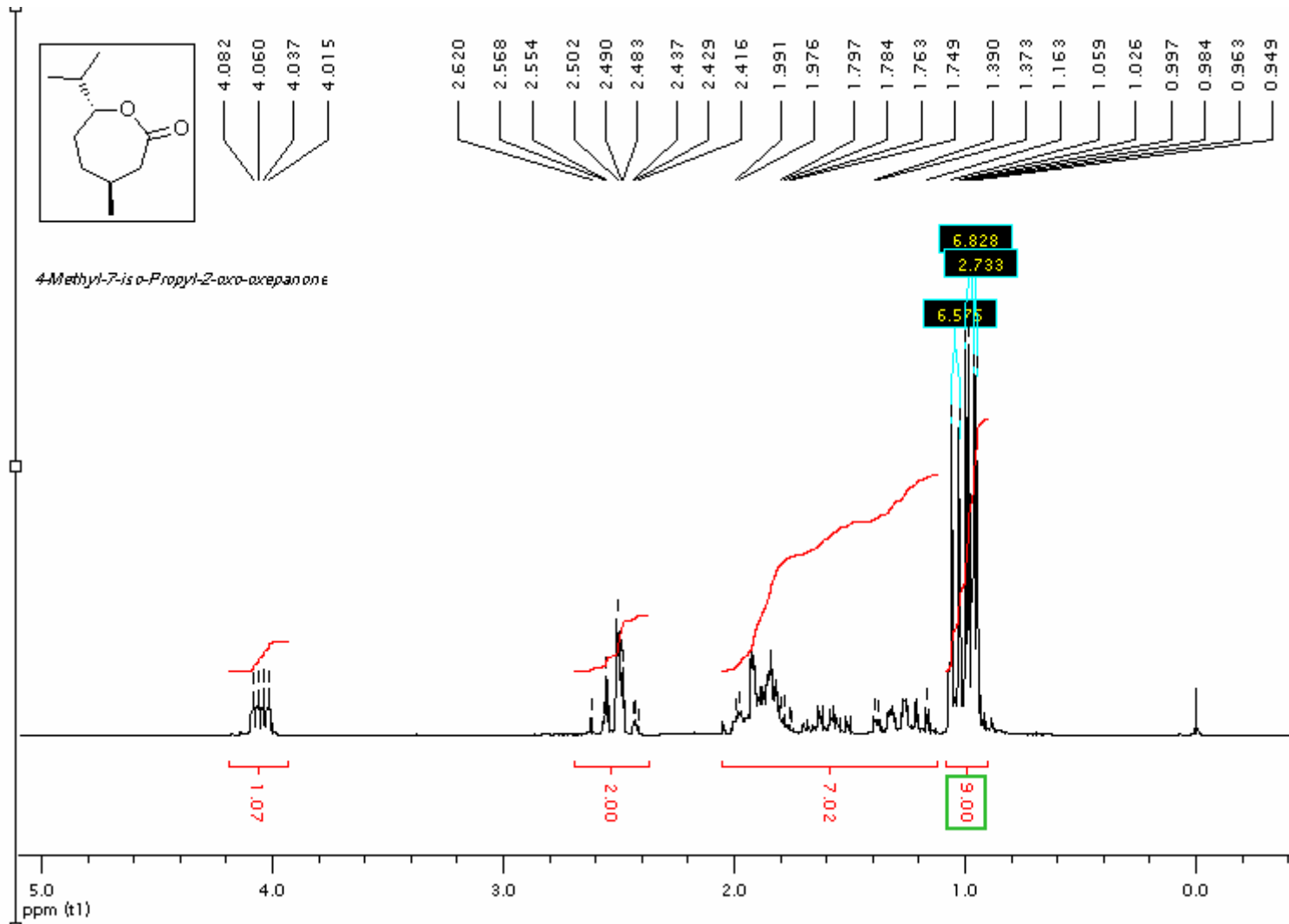
PC181-f1#816-821 RT: 7.89-7.92 AV: 6

T: {0;0} + c EI det=350.00 Full ms [ 50.00-400.00]

m/z = 49.60-400.40

| m/z   | Intensity | Relative |
|-------|-----------|----------|
| 52.98 | 315136.0  | 7.84     |
| 55.04 | 3442048.0 | 85.64    |
| 56.15 | 1924565.3 | 47.89    |
| 57.14 | 639669.3  | 15.92    |
| 67.02 | 348949.3  | 8.68     |
| 69.04 | 3855360.0 | 95.93    |
| 70.18 | 861194.7  | 21.43    |
| 71.17 | 255946.7  | 6.37     |
| 79.05 | 157373.3  | 3.92     |
| 81.07 | 4019029.3 | 100.00   |
| 82.22 | 335808.0  | 8.36     |
| 83.13 | 480266.7  | 11.95    |
| 84.18 | 86634.7   | 2.16     |
| 85.14 | 105576.0  | 2.63     |
| 98.11 | 3050453.3 | 75.90    |
| 99.16 | 3407872.0 | 84.79    |

<sup>1</sup>H NMR of the „normal“ lactone 4-Methyl-7-isopropyl-2-oxo-oxepanone



<sup>13</sup>C NMR of the „normal“ lactone 4-Methyl-7-isopropyl-2-oxo-oxepanone

