

Supporting Information Available

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Page 3 GC-MS of **1-d₀**

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Page 7 ^1H -NMR (500 MHz, CDCl_3) of **1-d₄**

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Page 10 ^1H -NMR (500 MHz, $\text{CS}_2/\text{C}_6\text{D}_6$) of **2-d₀**

Page 11 ^{13}C -NMR (500 MHz, $\text{CS}_2/\text{C}_6\text{D}_6$) of **2-d₀**

Page 12 MALDI TOF-MS of **2-d₀**

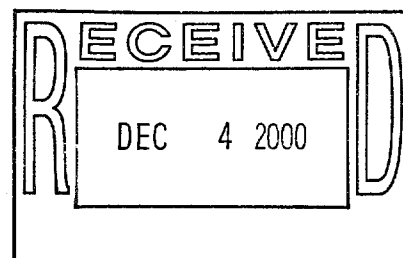
Page 13 ^1H -NMR (500 MHz, $\text{CS}_2/\text{C}_6\text{D}_6$) of **2-d₀/2-d₂**

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Page 15 ^1H -NMR (500 MHz, $\text{CS}_2/\text{C}_6\text{D}_6$) of **2-d₀/2-d₄**

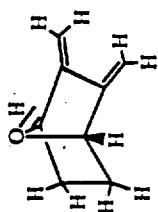
Page 16 MALDI TOF-MS of **2-d₀/2-d₄**

Page 17 Ab-Initio Theoretical Calculations. Fully Optimized Molecular Structures of the Folded and Extended Conformation of **2-d₀**



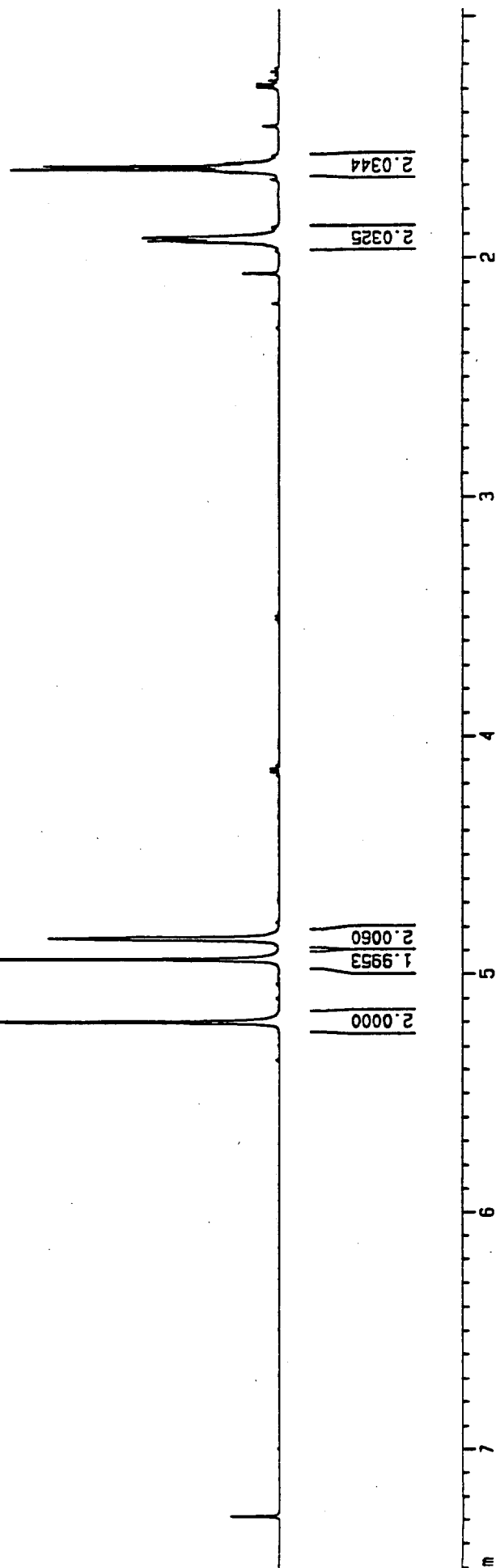
S1
¹H-NMR (500 MHz, CDCl₃) of 1-d₀

2.06398
 1.93579
 1.93015
 1.92231
 1.91556
 1.91055
 1.64452
 1.63275
 1.61880
 1.60633

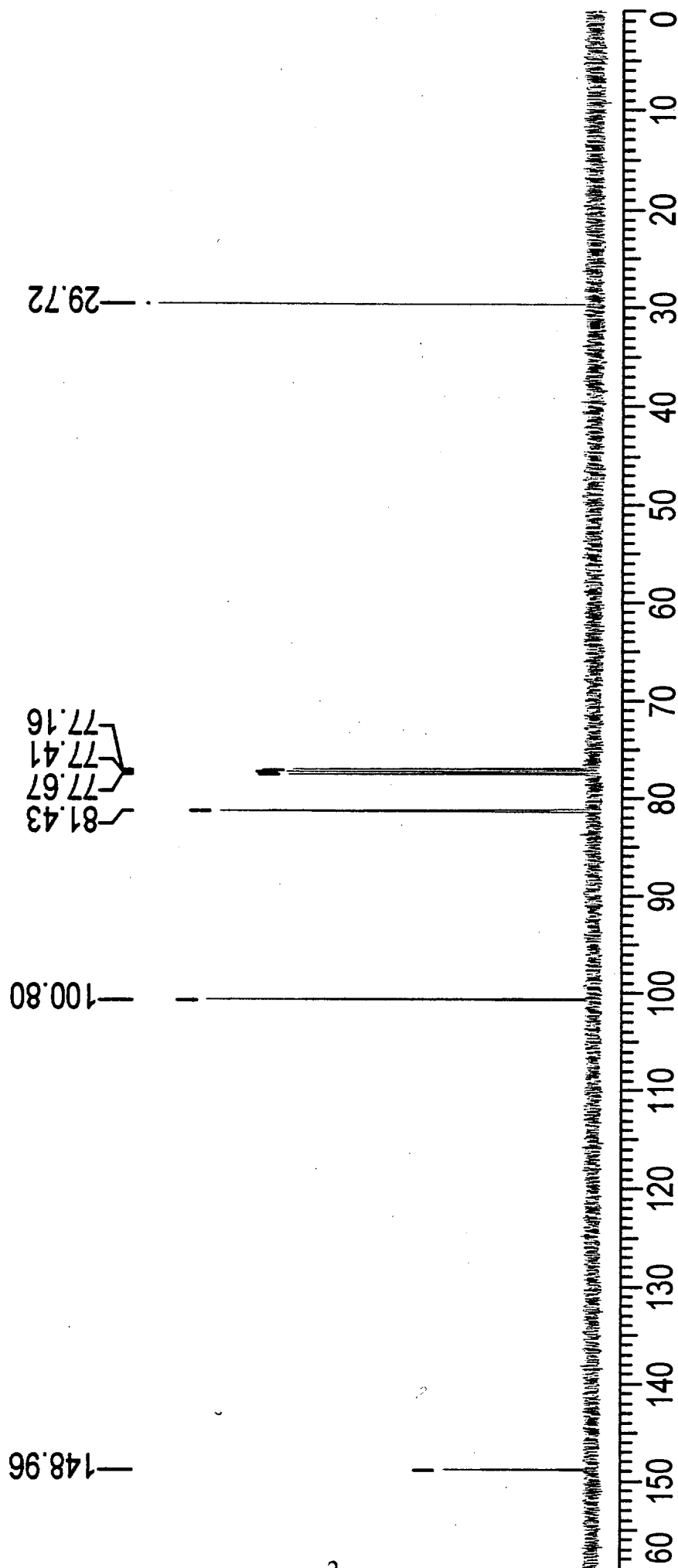


5.20288
 4.94281
 4.85250
 4.84809

7.28605



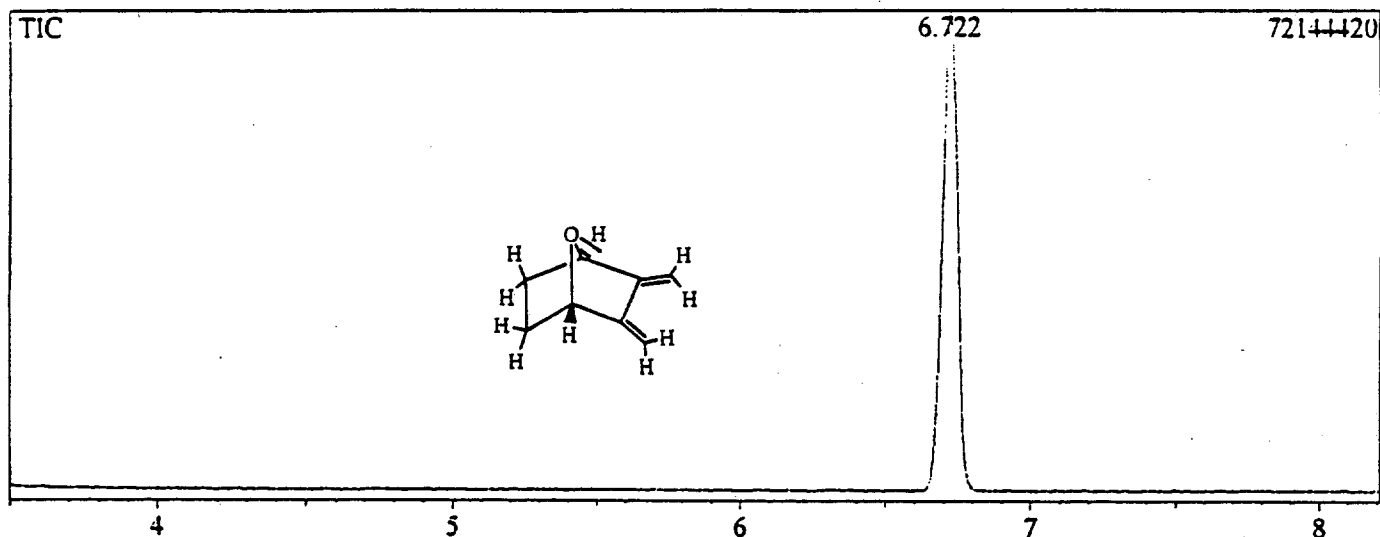
S2
 ^{13}C -NMR (500 MHz, CDCl_3) of 1-d₀



Dilution Factor : 1

Method File Name : NIKOS.MET

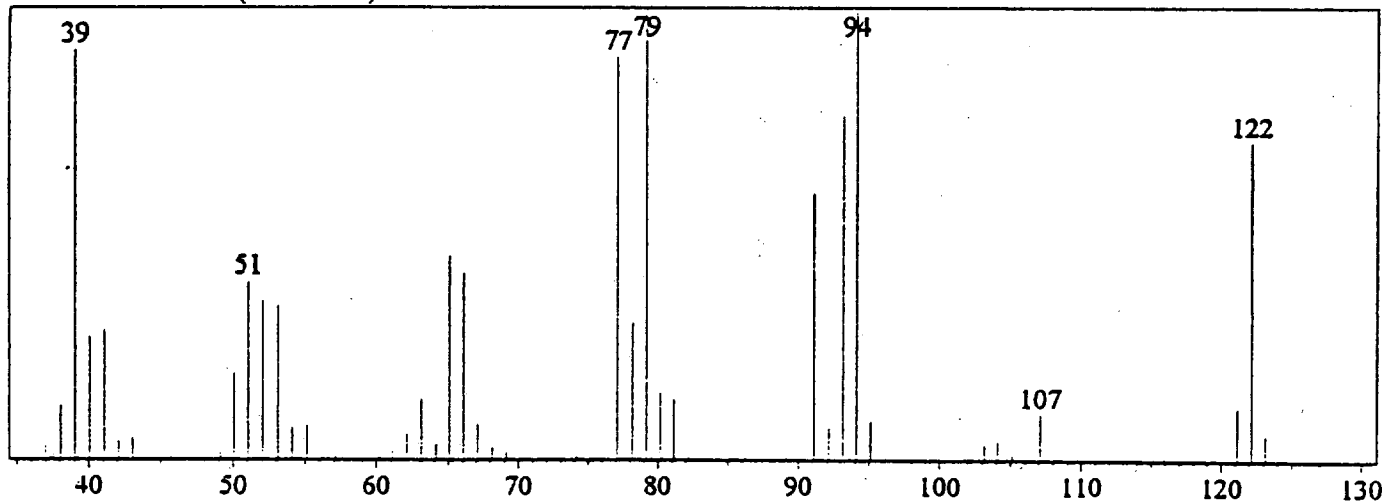
S3
GC-MS of 1-d₀



Scan # : (379 - 397) B.G. Scan # : (359 - 378)

Mass Peak # : 81 Ret. Time : (6.650 - 6.800)

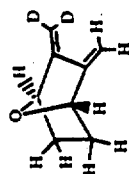
Base Peak : 79.15 (2507477)



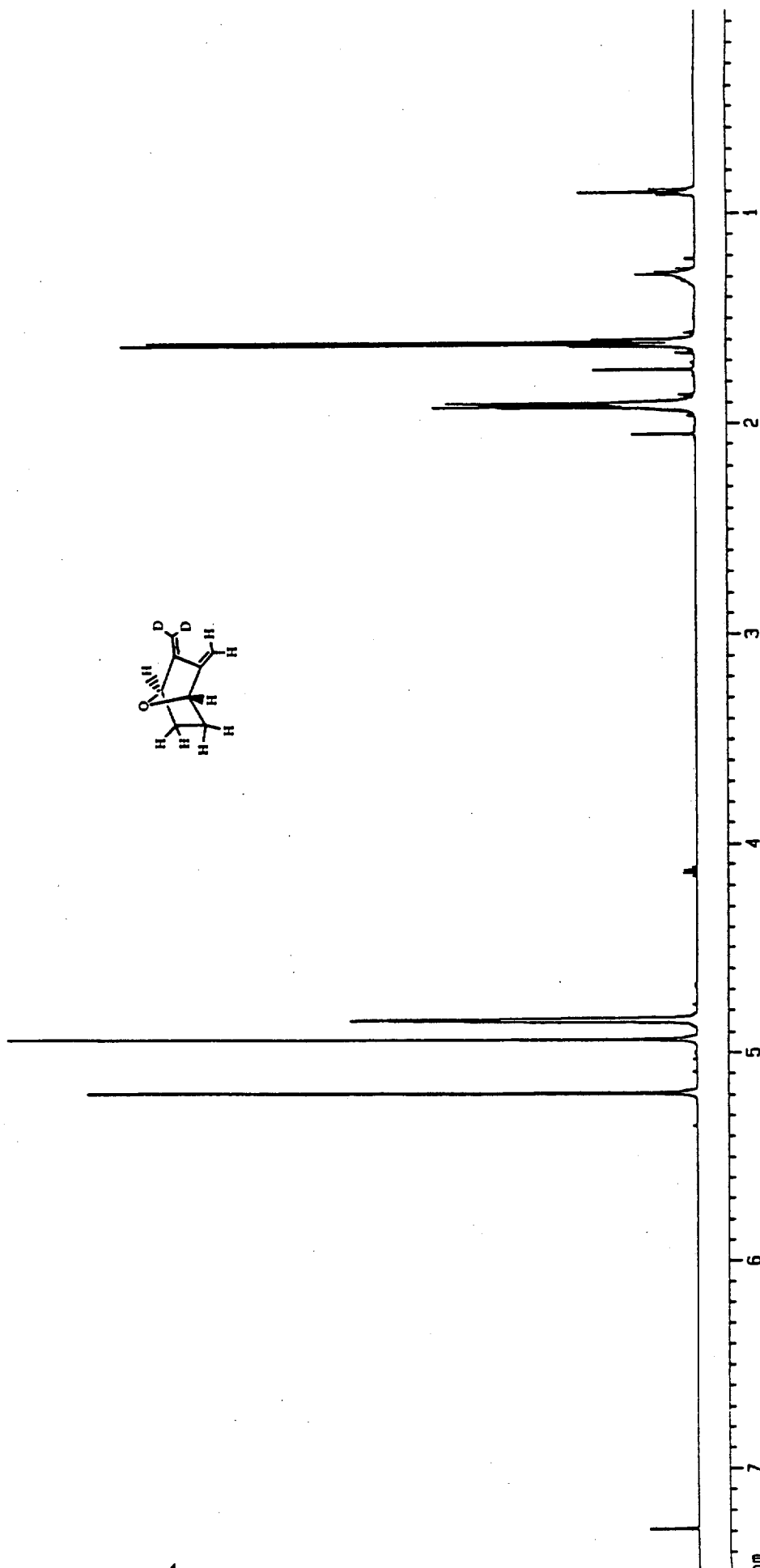
S4

¹H-NMR (500 MHz, CDCl₃) of 1-d₂

0.90135
1.59491
1.60048
1.60371
1.60723
1.62139
1.62779
1.63322
1.74233
1.89545
1.89938
1.90460
1.91132
1.91361
1.91881
1.92273
1.92506

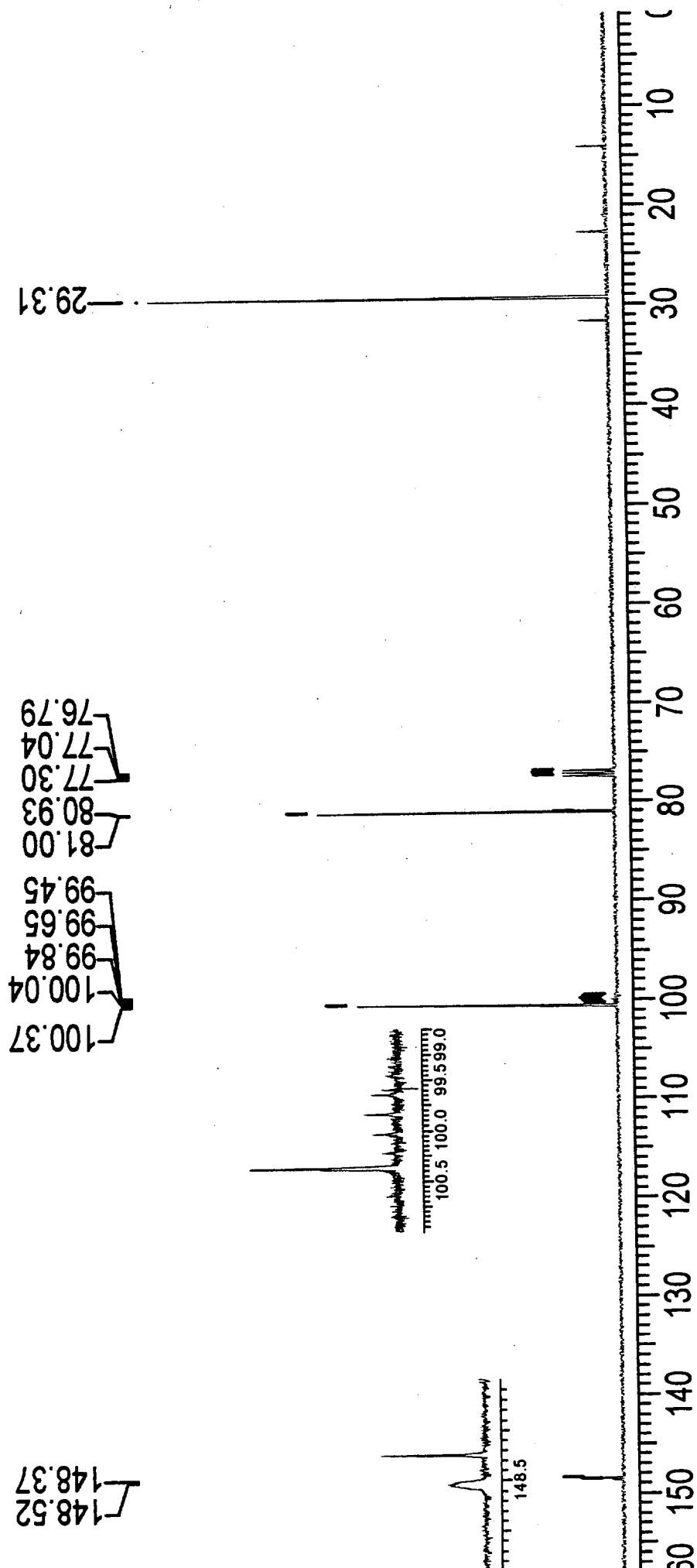


4.84048
4.84291
4.84487
4.84679
4.93457
5.19085
5.19251

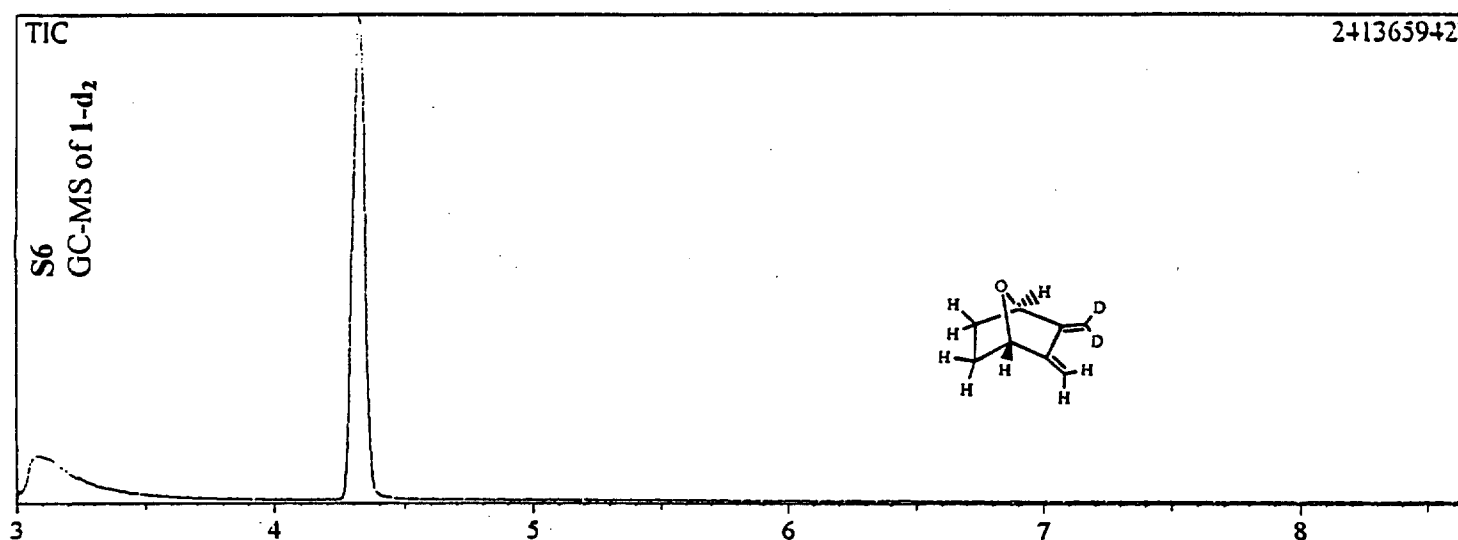


S5

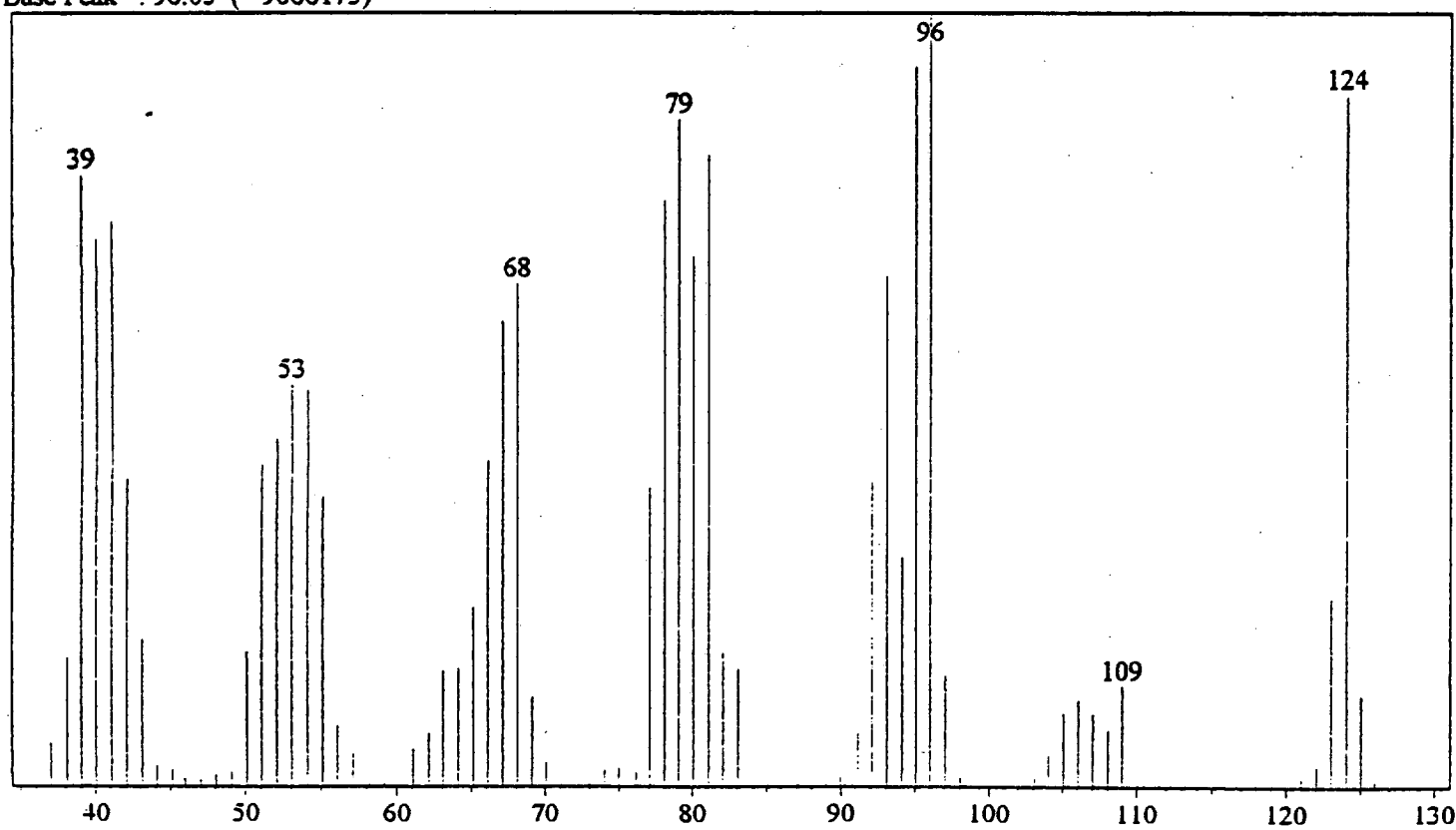
^{13}C -NMR (500 MHz, CDCl_3) of 1-d₂



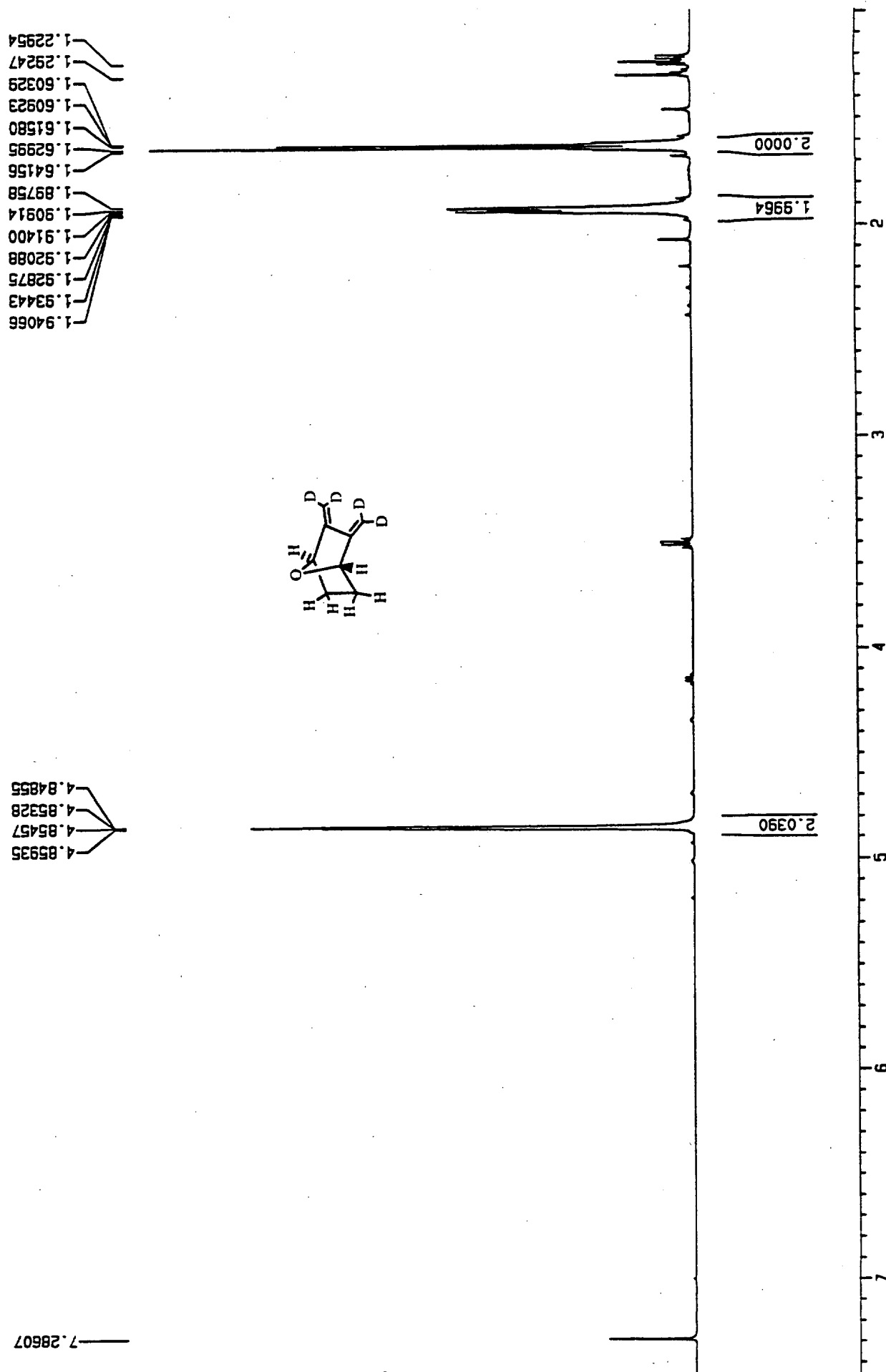
Dilution Factor : 1
 Method File Name : NIKOS.MET
 Vial No. : 1



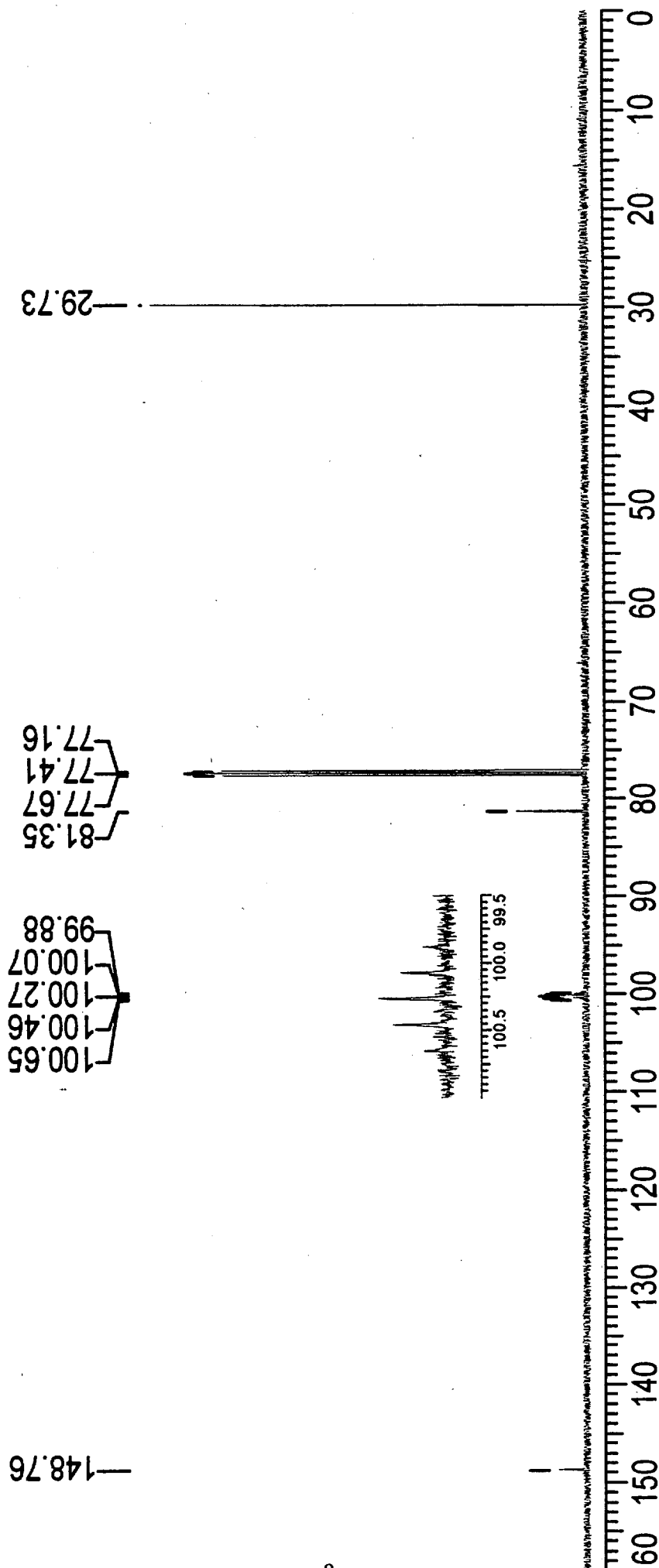
Scan # : (157 - 164) B.G. Scan # : 154
 Mass Peak # : 90 Ret. Time : (4.300 - 4.358)
 Base Peak : 96.05 (9066175)



S7
¹H-NMR (500 MHz, CDCl₃) of 1-d₄

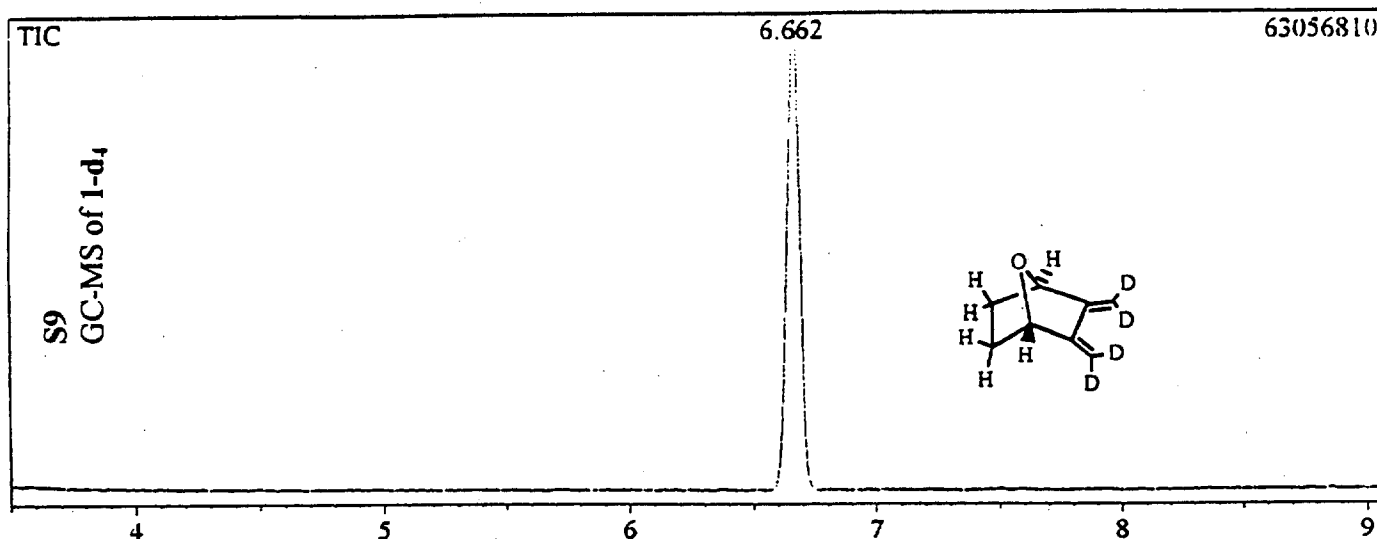


S8
 ^{13}C -NMR (500 MHz, CDCl_3) of 1-d₄



Dilution Factor : 1

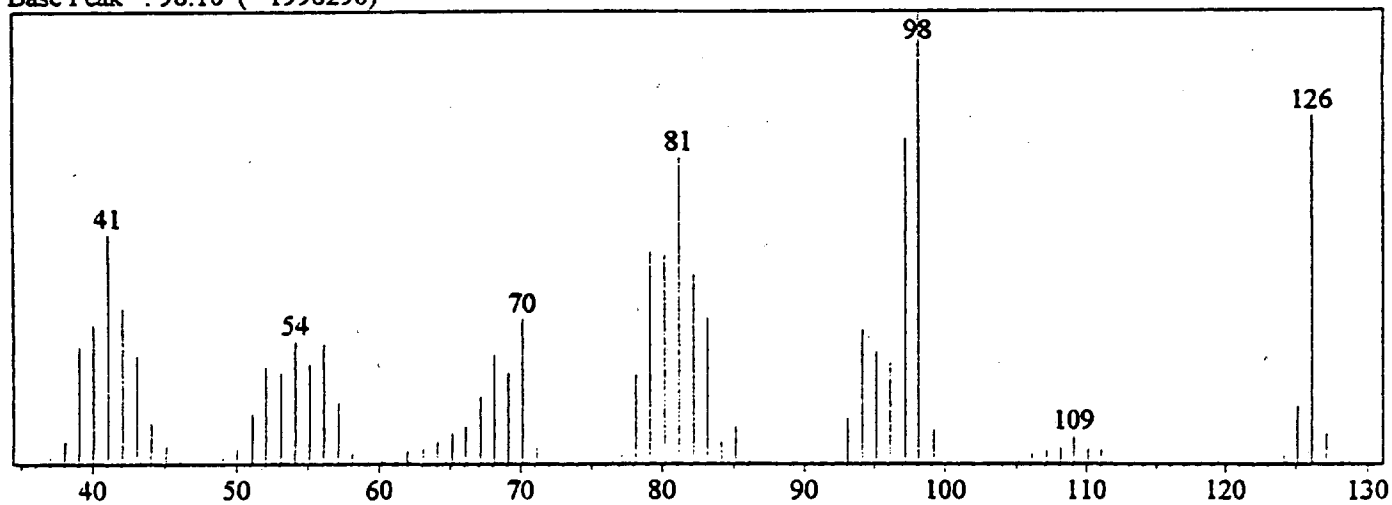
Method File Name : NIKOS.MET



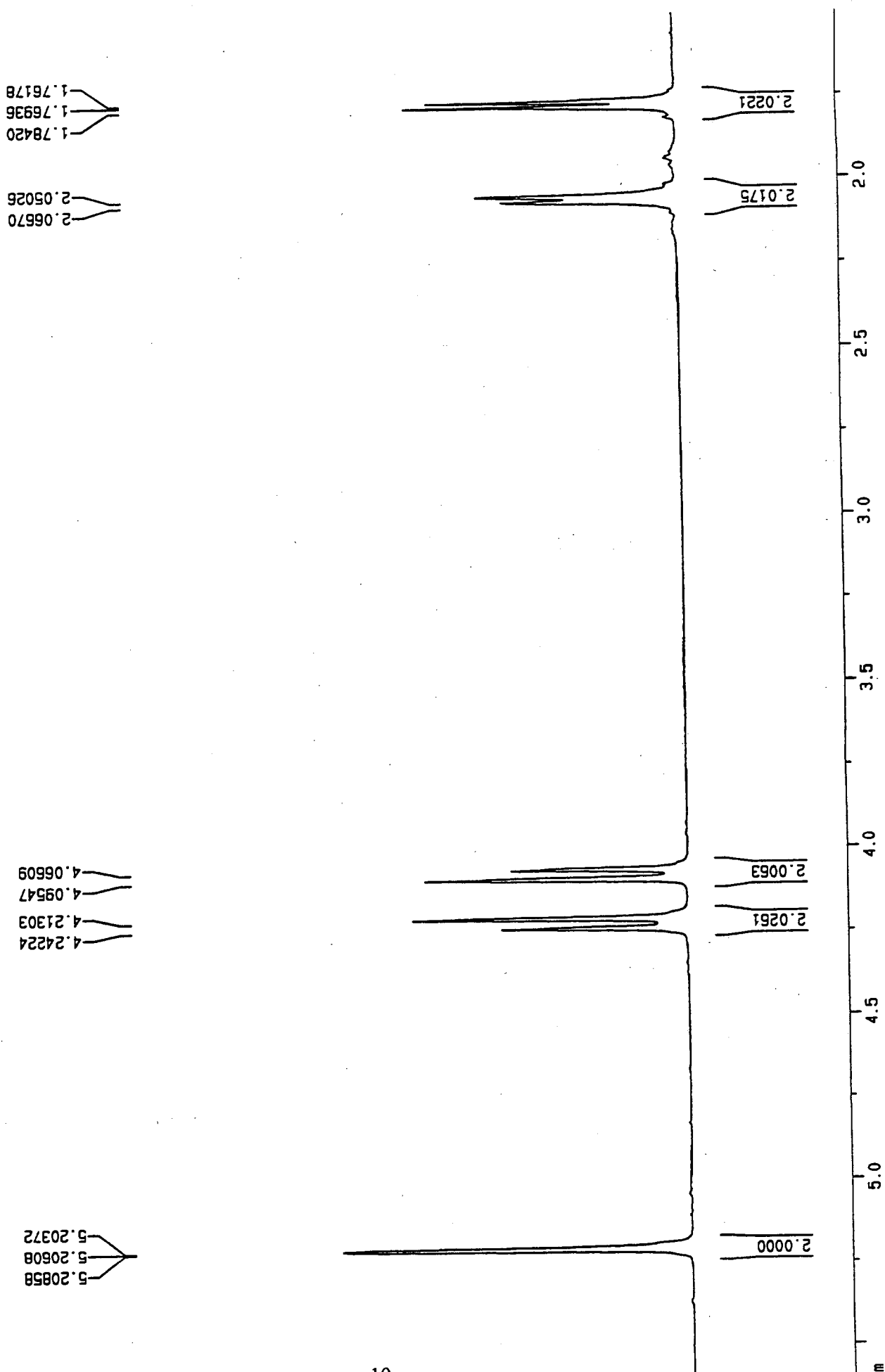
Scan # : (372 - 390) B.G. Scan # : (345 - 371)

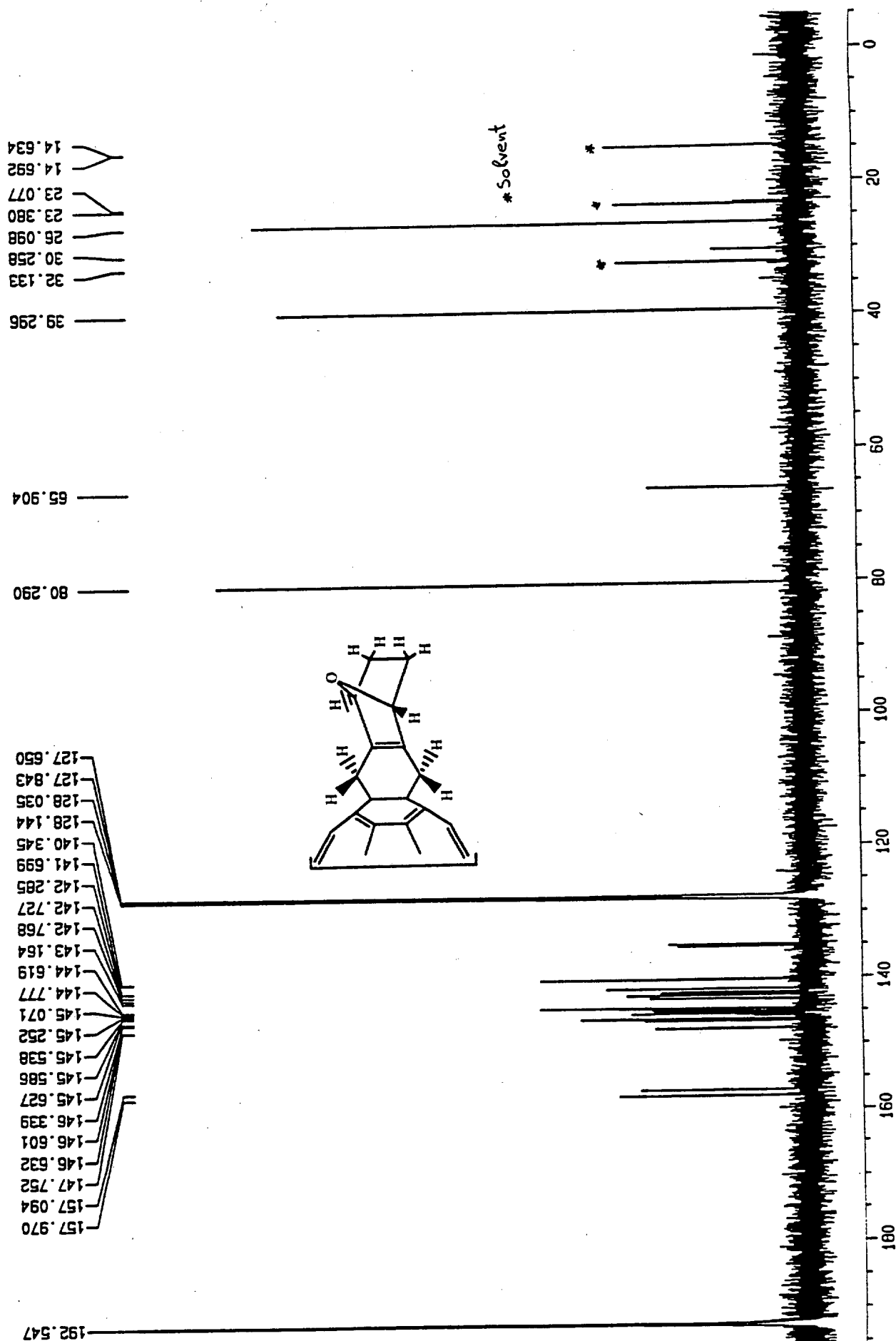
Mass Peak # : 92 Ret. Time : (6.592 - 6.742)

Base Peak : 98.10 (1996290)



S10
¹H-NMR (500 MHz, CS₂/C₆D₆) of 2-d₀





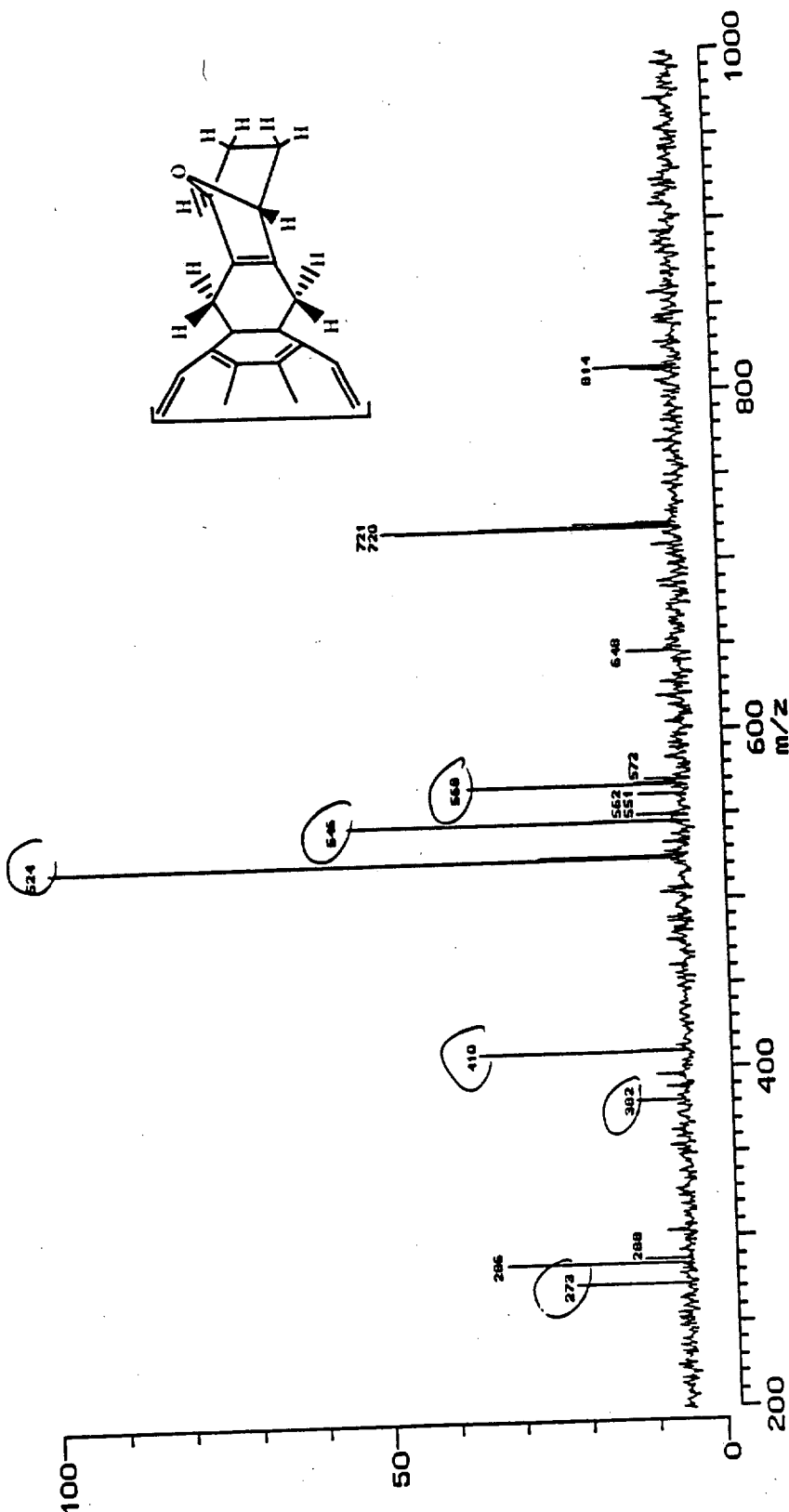
S12
MALDI TOF-MS of 2-d₀

Date: 27-AUG-1999
Time: 11:13:59
Mode: Positive
Scans: 20
Scale: 353.7928

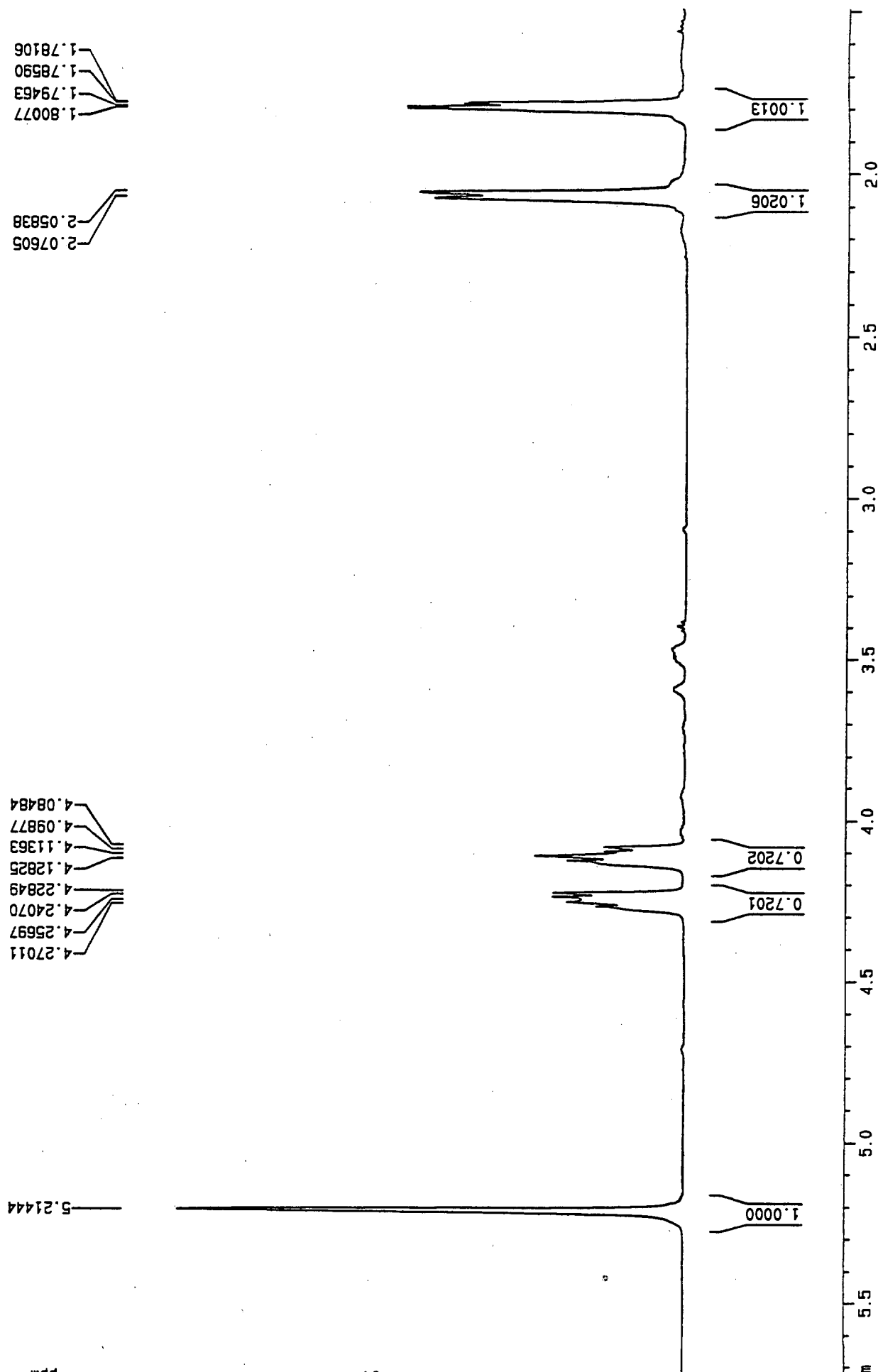
IonSpec HiResMALDI

File: c:\ionspec\ftdata\KC990827.017

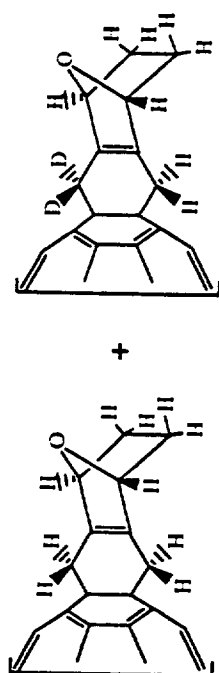
kc99v



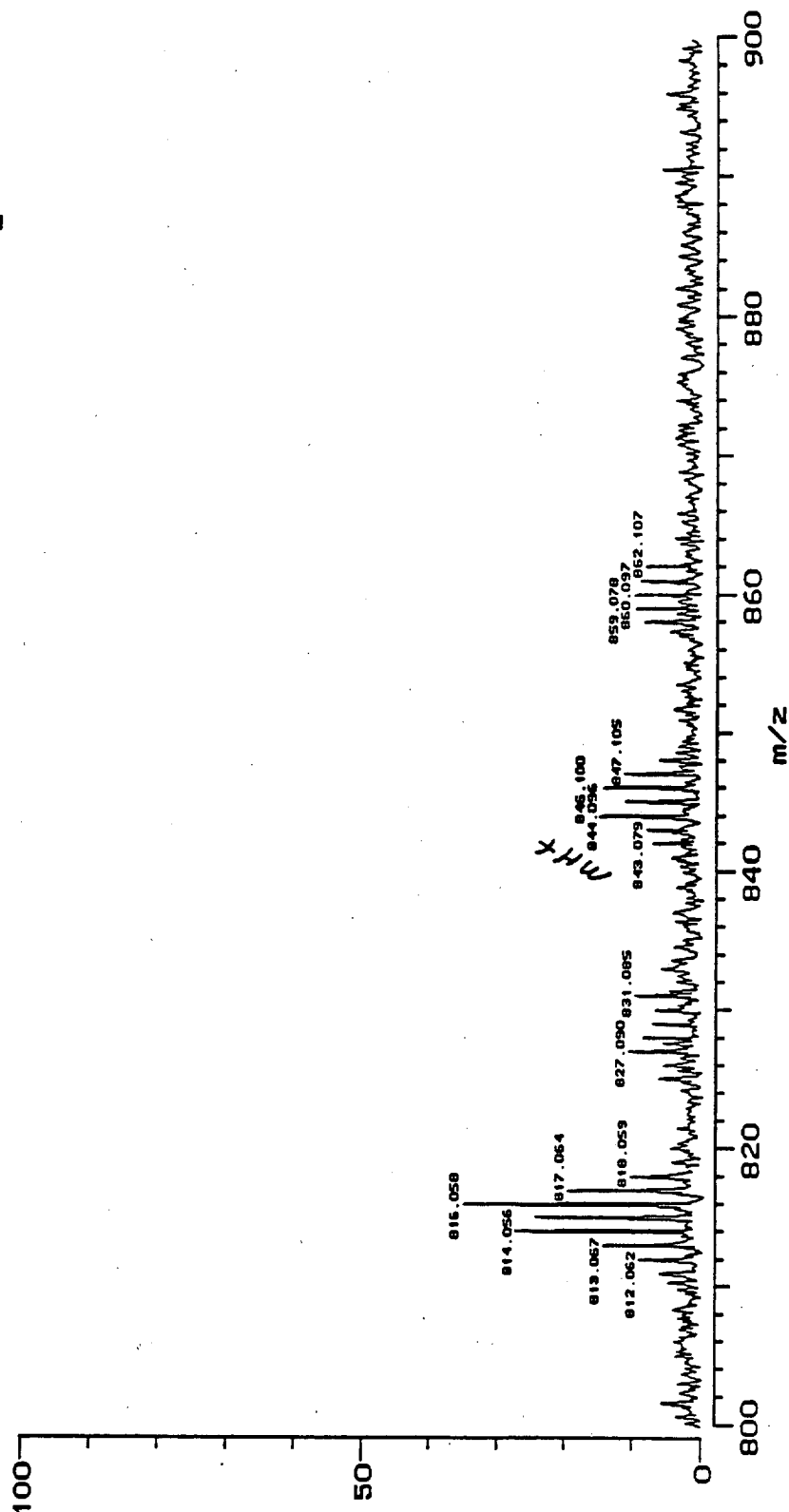
S13
¹H-NMR (500 MHz, CS₂/C₆D₆) of 2-d₂/2-d₂



S14
MALDI TOF-MS of 2-d₀/2-d₂

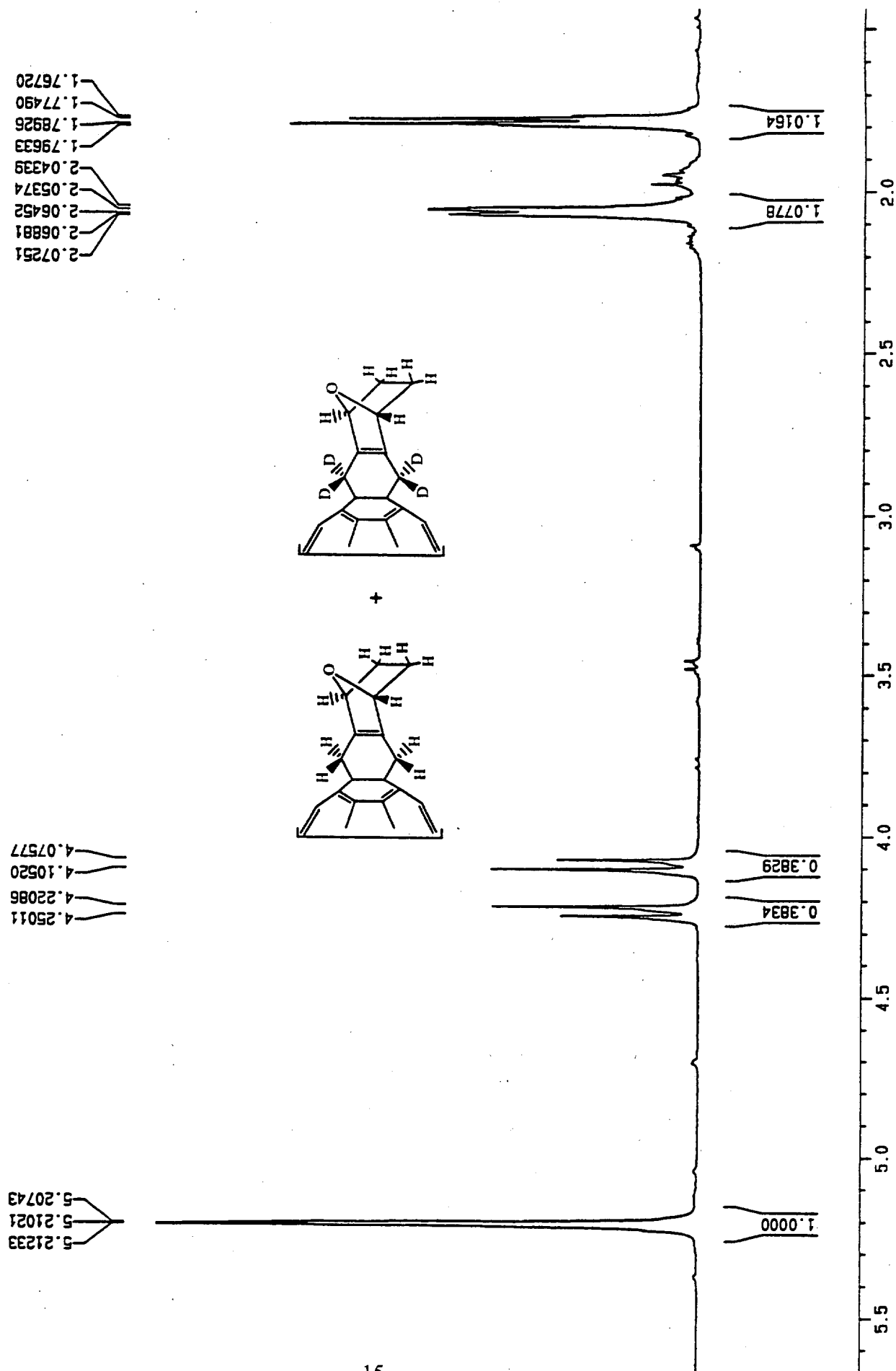


IonSpec HiResMALDI
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kc9ob



S15

¹H-NMR (500 MHz, CS₂/C₆D₆) of 2-d₀/2-d₄

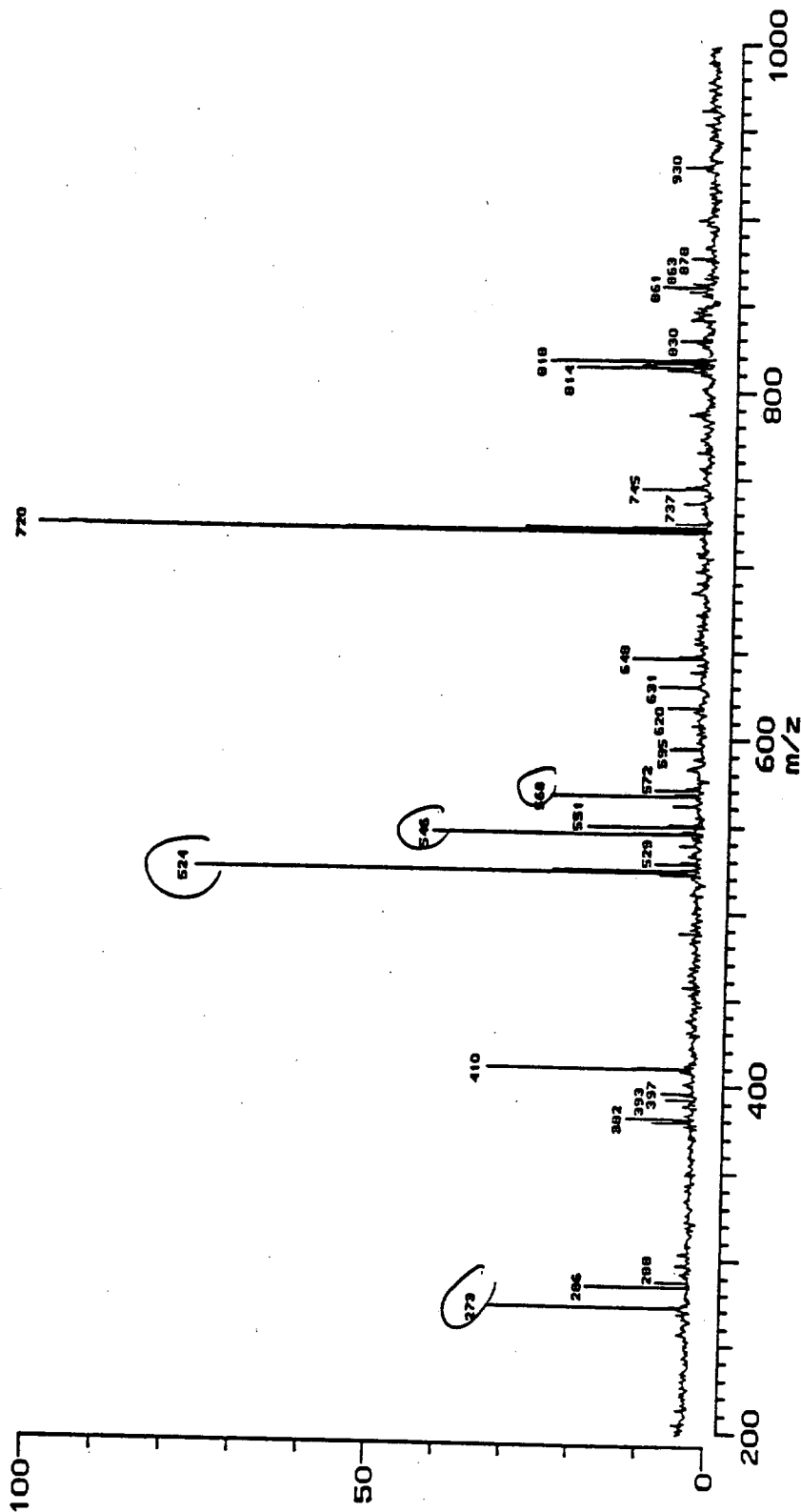
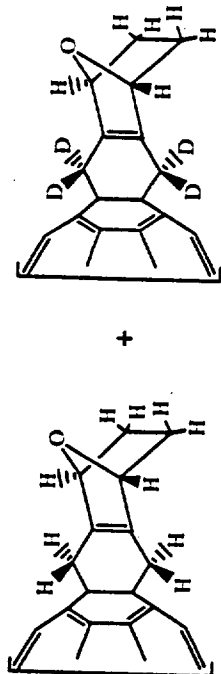


S16
MALDI TOF-MS of 2-d₀/2-d₄

IonSpec HiResMALDI

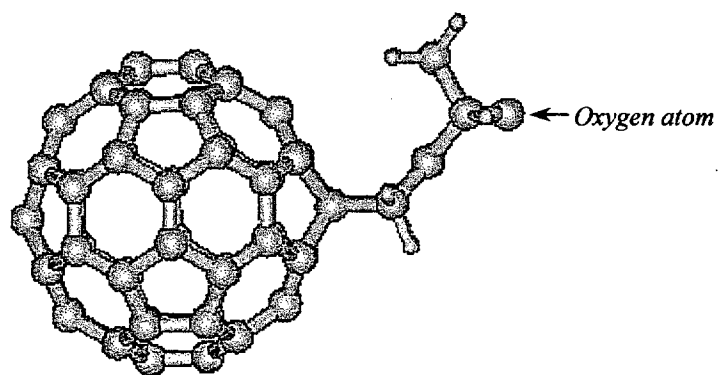
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kc9lk



S17

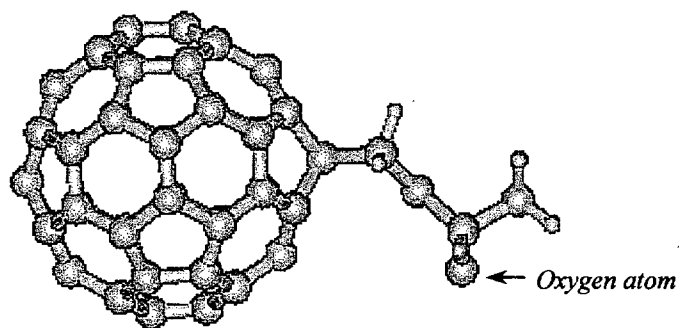
Ab-Initio Theoretical Calculations. Fully Optimized Molecular Structures of the Folded and Extended Conformation of **2-d₀**.



Folded Conformation

HF/3-21G

Total Energy = -2640.535947 Hy



Extended Conformation

HF/3-21G

Total Energy = -2640.535093 Hy