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Report of Analytical Services

Submitted To:

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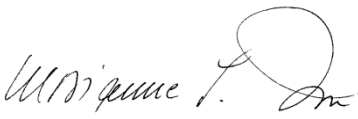
Attention: MR. DON WRIGHT

We are pleased to provide the enclosed analytical results for the following project.
Should you have any questions regarding the methods and/or results, please feel free to write or call.

Client Project:	Identify one unknown peak in one data file
Description:	Customer data
Laboratory Project:	S845
Project Objective:	Data Review
Date received:	8/14/2015
Date completed:	8/17/2015
Report date:	8/17/2015

Verified_____
Stephen R. Shrader, Ph.D.



Approved_____
Marianne L. Shrader, President

Enclosure(s)

Contents

INTRODUCTION

The data file MAGO166.D was evaluated in order to identify a peak eluting at 12.8 minutes, on the back edge of a limonene peak (RT 12.78) and before a 1,8-cineole peak (RT 12.96).

PROCEDURES

The data file was evaluated as follows.

- Total Ion Current and selected mass chromatograms were plotted.
- Averaged spectra (three mass spectra around each peak retention time) with the background subtracted were plotted.
- Library searches were performed with the NIST 2008 data base.
- Spectra not resulting in a good library match were interpreted by standard rules.

RESULTS

The chromatogram (Figure 1) contains four major peaks and several smaller peaks. The identities of the five strongest peaks are confirmed by comparing their mass spectra to reference mass spectra in the NIST08 database.

Table 1 Five largest peaks in chromatogram of eomem fc

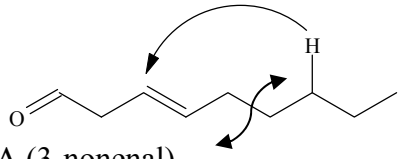
Compound ID	RT(Min.)	Figure
Limonene	12.78	2
m-Cymene	13.21	3
Hemellitol	13.81	4
Dichlorobenzene	14.94	5
2-Ethyl-1-hexanol	15.58	6

The identity of 1,8-cineole (RT 12.96) is also confirmed in this manner (Figure 7).

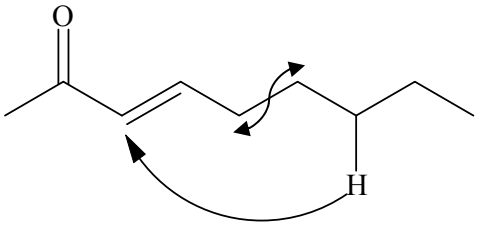
A component is also detected on the back end of the limonene peak (Figure 8). Its mass spectrum is shown in Figure 9. No reasonable matches to this spectrum with reference spectra in the NIST08 database are found.
This spectrum is consistent with a compound having molecular weight 140, fragmenting readily by loss of CH_3(giving fragment mass 125), C_2H_5(giving fragment mass 111), C_3H_7(giving fragment mass 97) and C_4H_8(giving fragment mass 84),
Two possible elemental compositions are considered: $C_{10}H_{20}$ and $C_9H_{16}O$.
The hydrocarbon $C_{10}H_{20}$ would be expected to give more intense low-mass fragments (see Figures 10 –16 for several examples of $C_{10}H_{20}$ mass spectra).
Close examination of the isotope peak intensity for the molecular ion (mass 140) also favors the $C_9H_{16}O$ formula (see Figures 17 – 18 and Tables 2 - 5).
Several reference spectra from the NIST08 database are shown in Figures 19 – 23. Although none closely match the spectrum of the unknown component, they show the fragmentation-directing power of the oxygen atom.
Based on the fragments observed in the mass spectrum of Figure 9, the structures A - F can be considered.
These structures can all lose the simple C_nH_{2n+1} fragments, and the important McLafferty rearrangement to lose C_4H_8.

Other isomers are also possible.

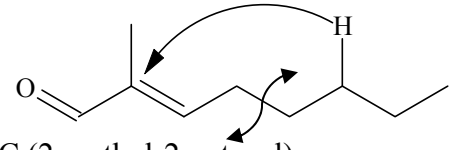
Please also note the reference spectrum of 2-butyl-cyclohexane (Figure 24). This $C_{10}H_{18}O$ compound fragments very readily by loss of the C_4H_8 unit.
Also note the reference spectrum of 2-pentyl-cyclopentanone (Figure 25).



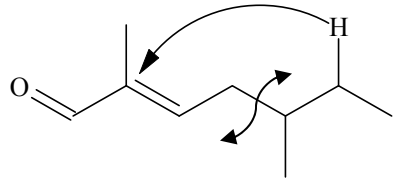
A (3-nonenal)



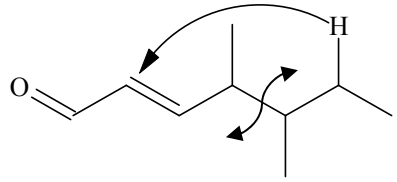
B (3-nonene-2-one)



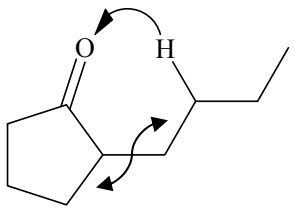
C (2-methyl-2-octenal)



D(2,5-dimethyl-2-heptenal)



E(4,5-dimethyl-2-heptenal)



F(2-butyl-cyclopentanone)

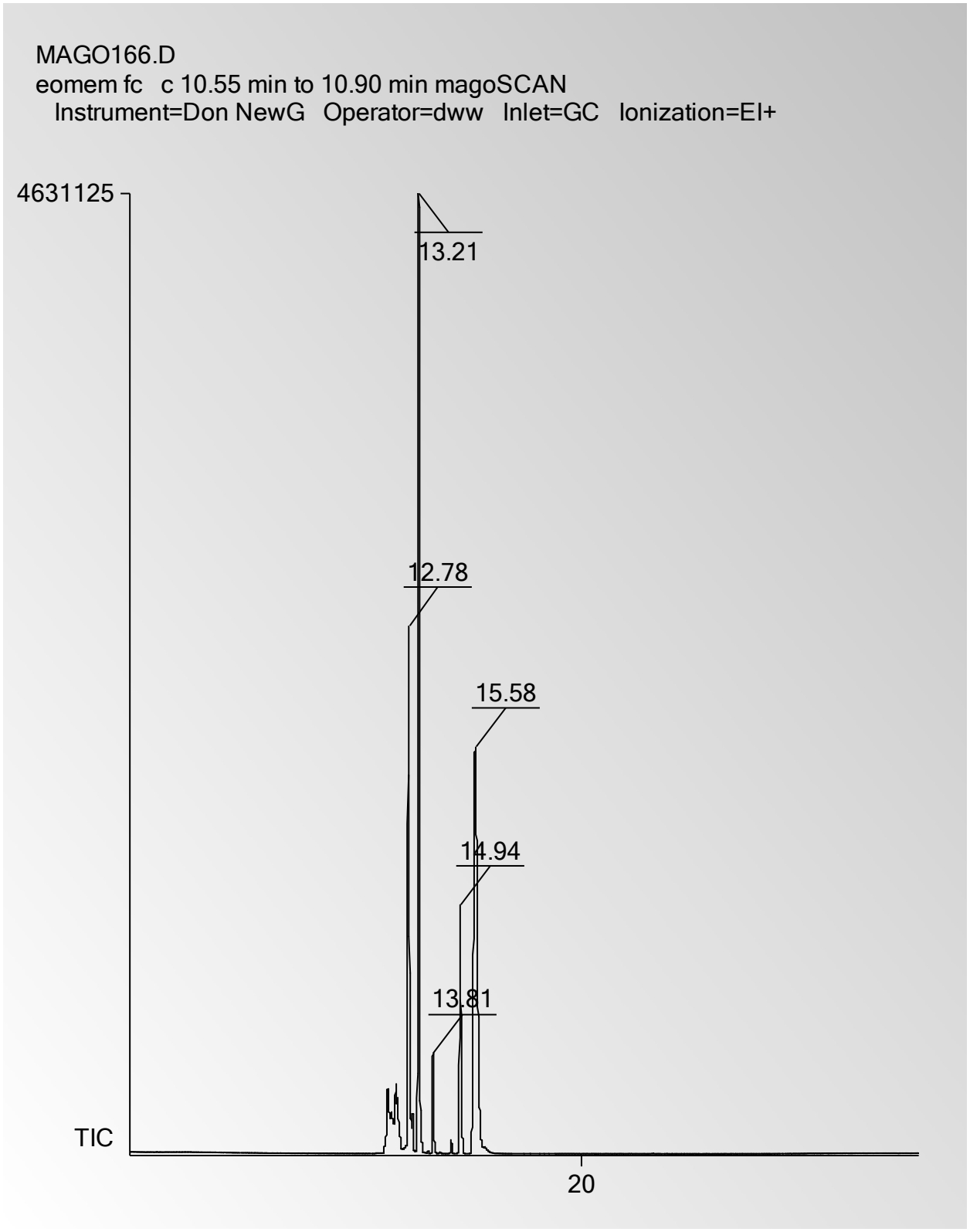


Figure 1 Chromatogram for eomem fc

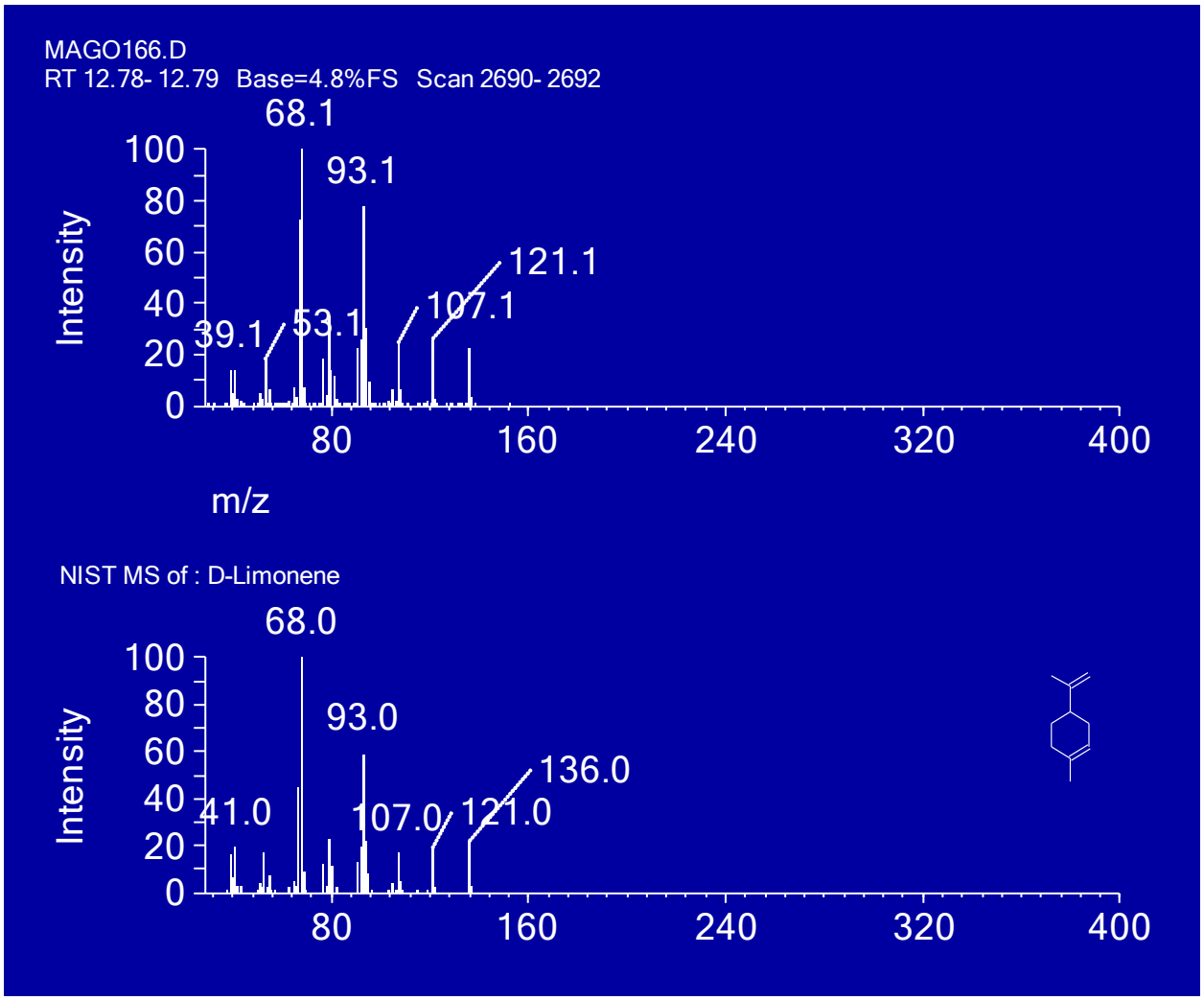


Figure 2 MS of eomem fc at RT 12.78- 12.79 and NIST MS of : D-Limonene Match factor 95

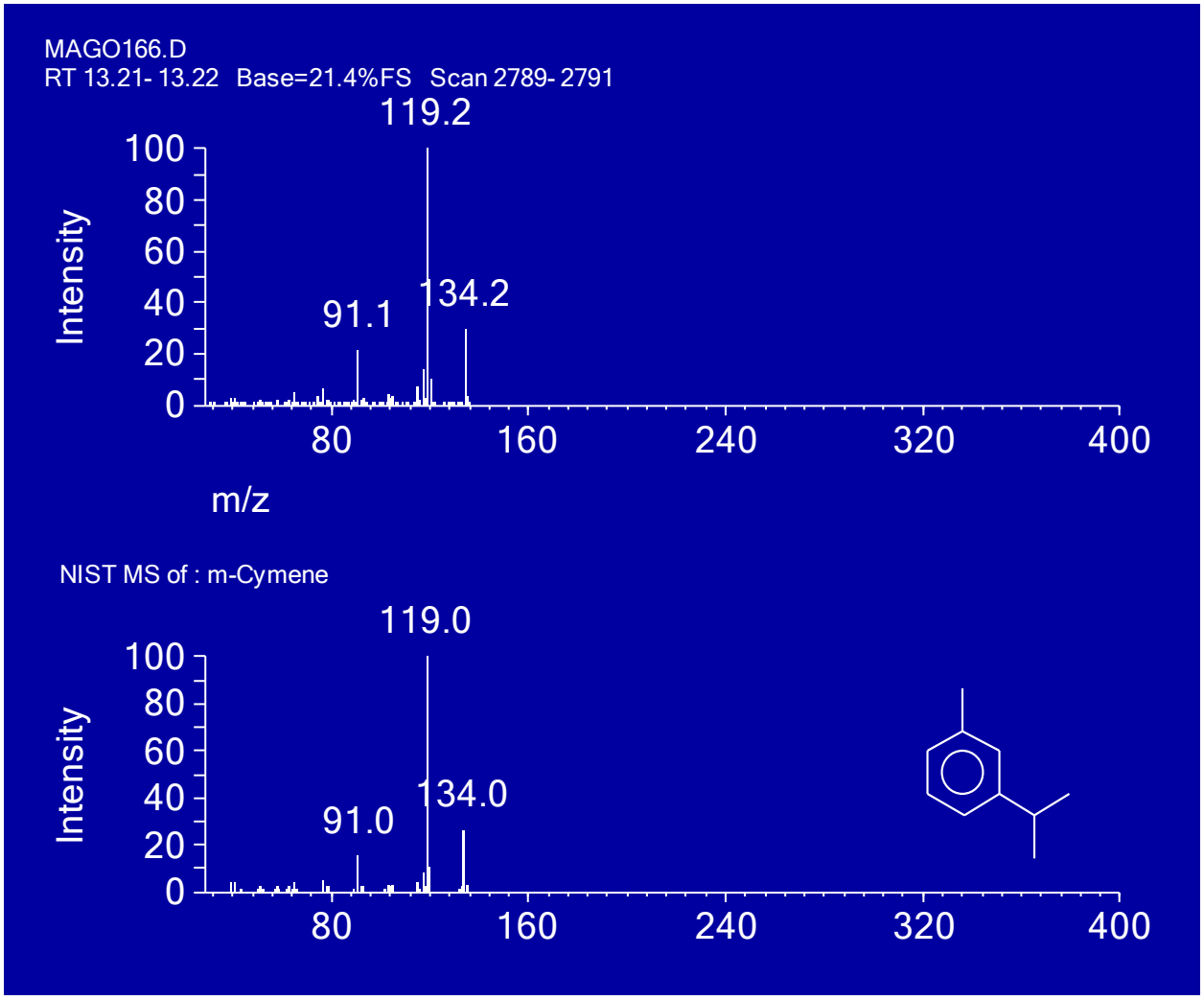


Figure 3 MS of eomem fc at RT 13.21- 13.22 and NIST MS of : m-Cymene Match factor 92.4

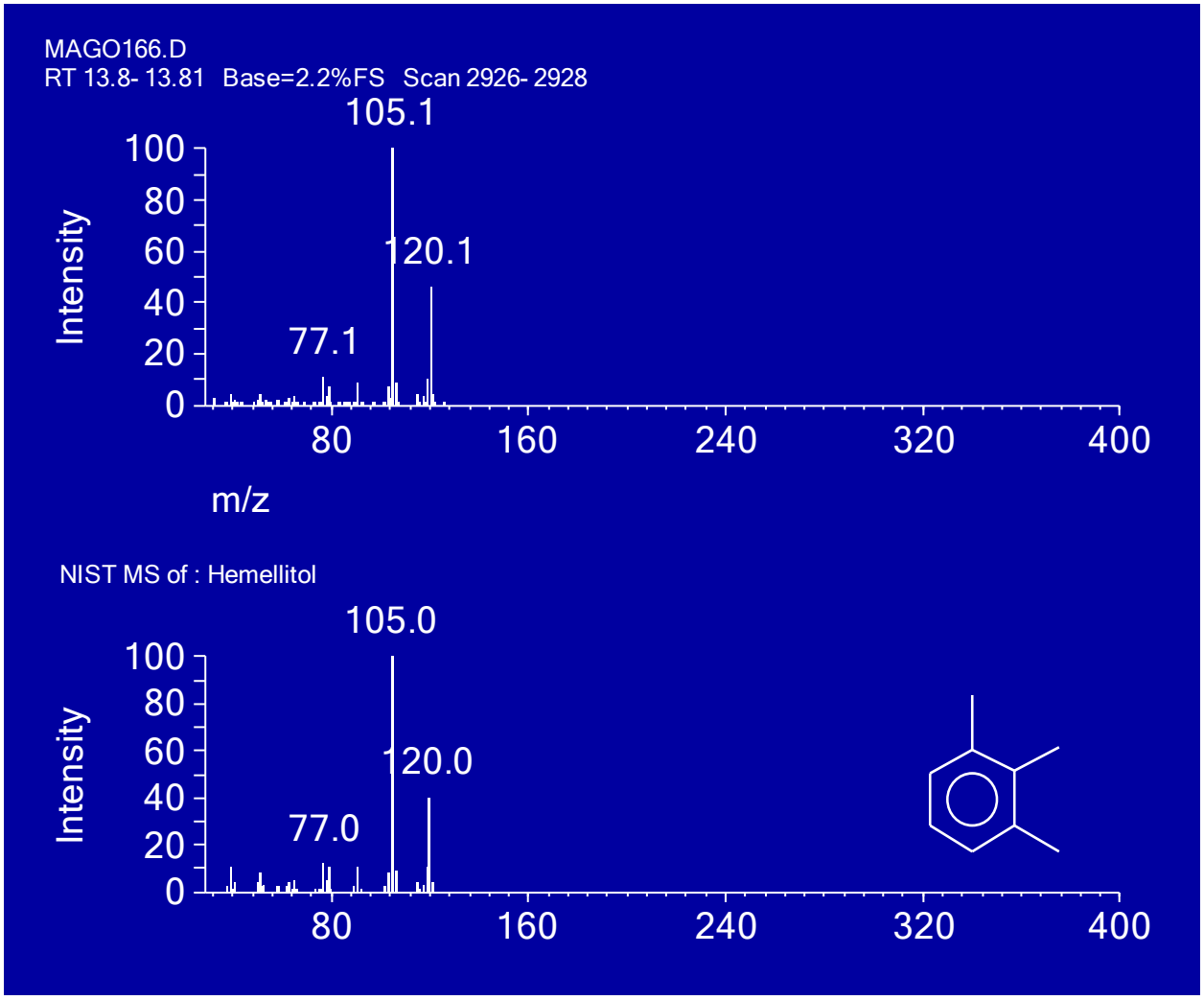


Figure 4 MS of eomem fc at RT 13.8- 13.81 and NIST MS of : Hemellitol Match factor 94.7

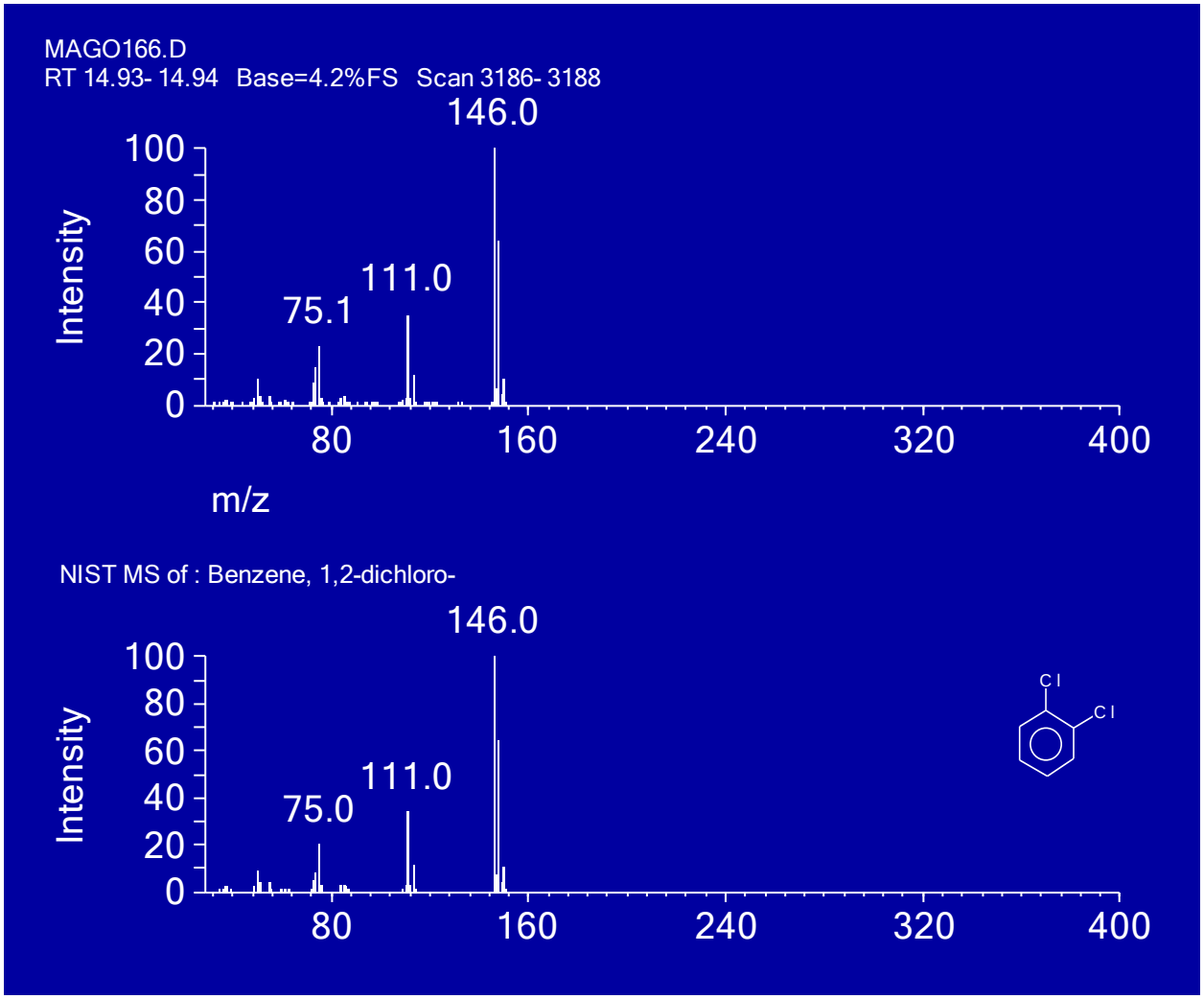


Figure 5 MS of eomem fc at RT 14.93- 14.94 and NIST MS of : Benzene, 1,2-dichloro- Match factor 96.9

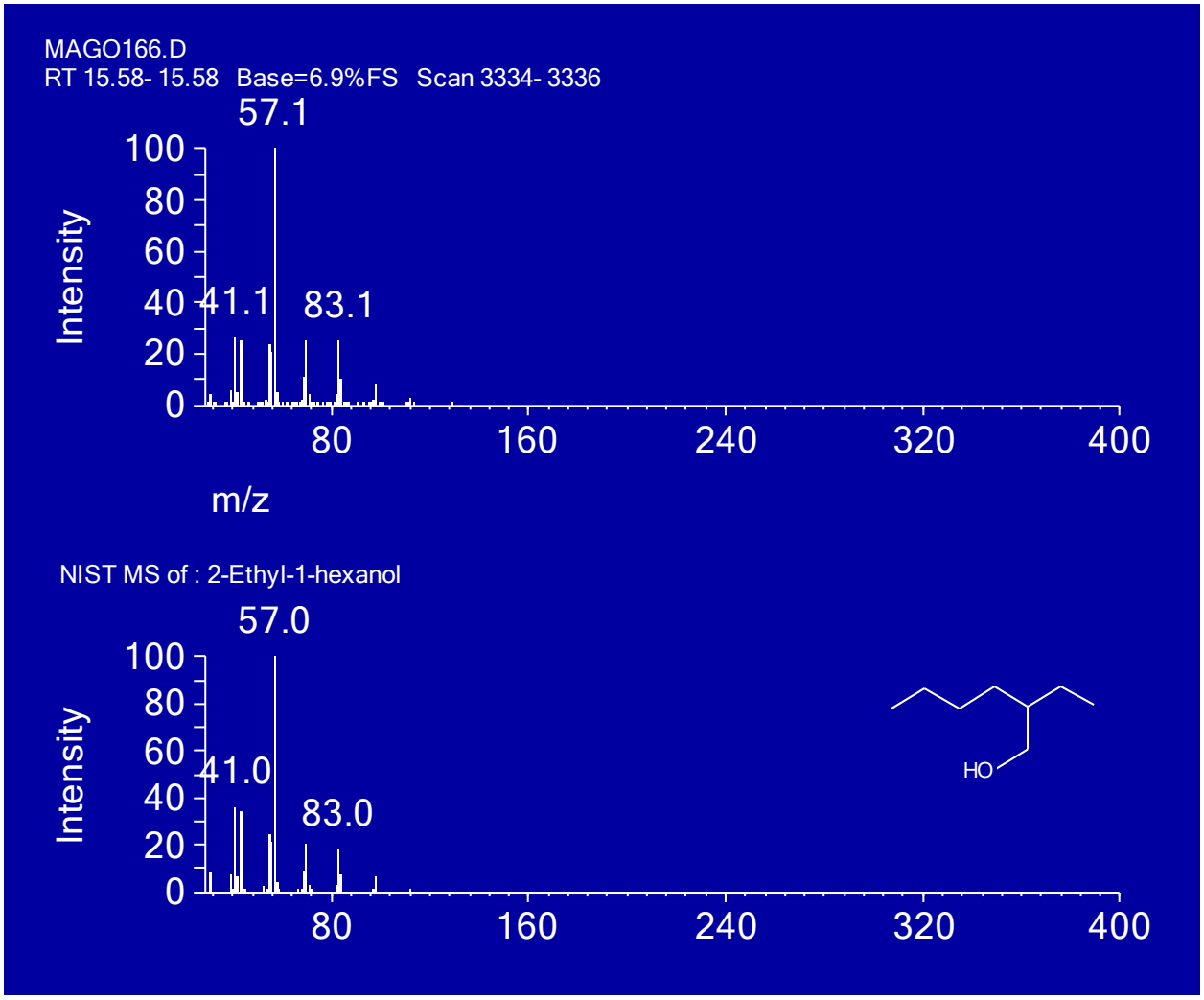


Figure 6 MS of eomem fc at RT 15.58- 15.58 and NIST MS of : 2-Ethyl-1-hexanol Match factor 95.2

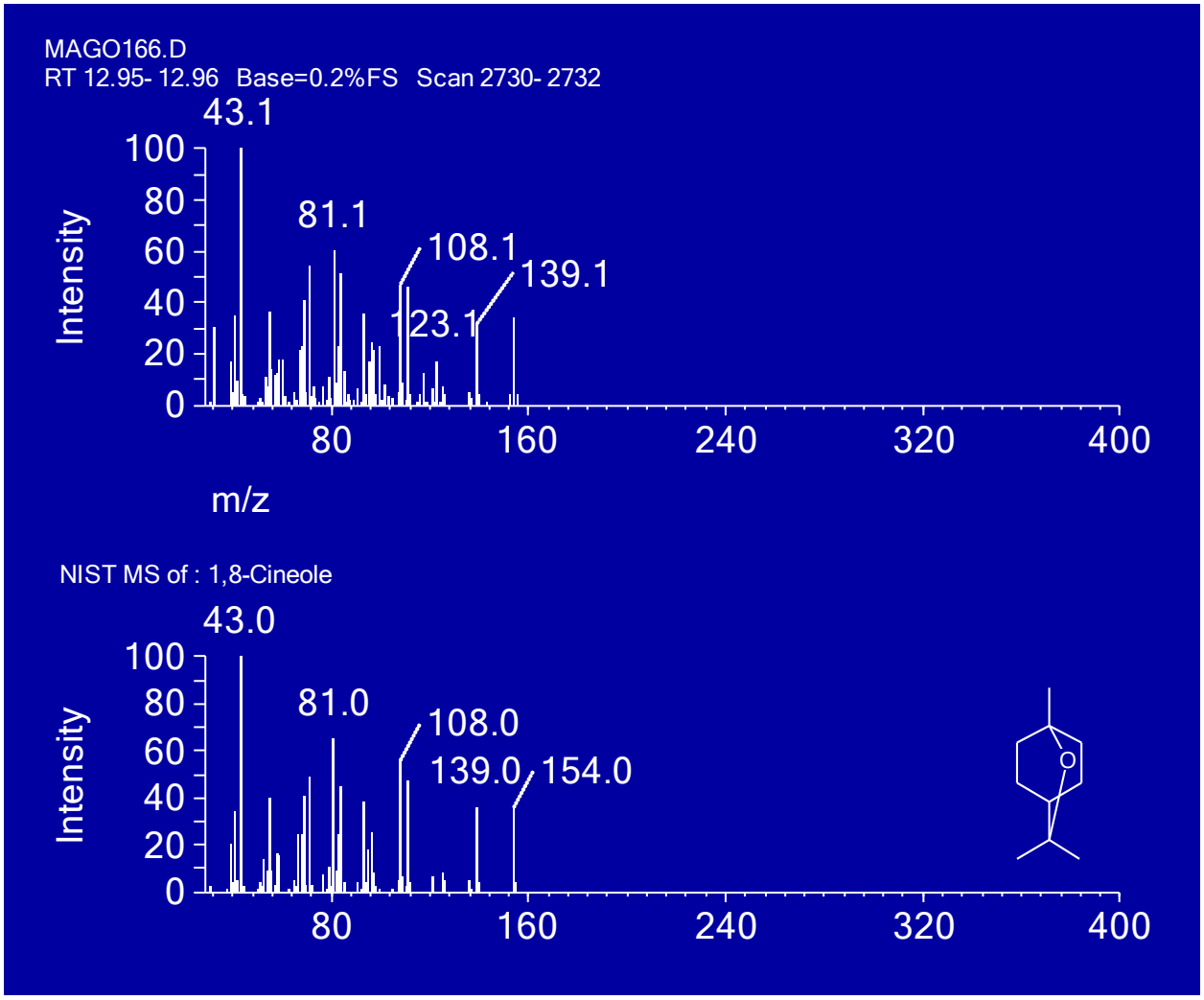


Figure 7 MS of eomem fc at RT 12.95- 12.96 and NIST MS of : 1,8-Cineole Match factor 82.2

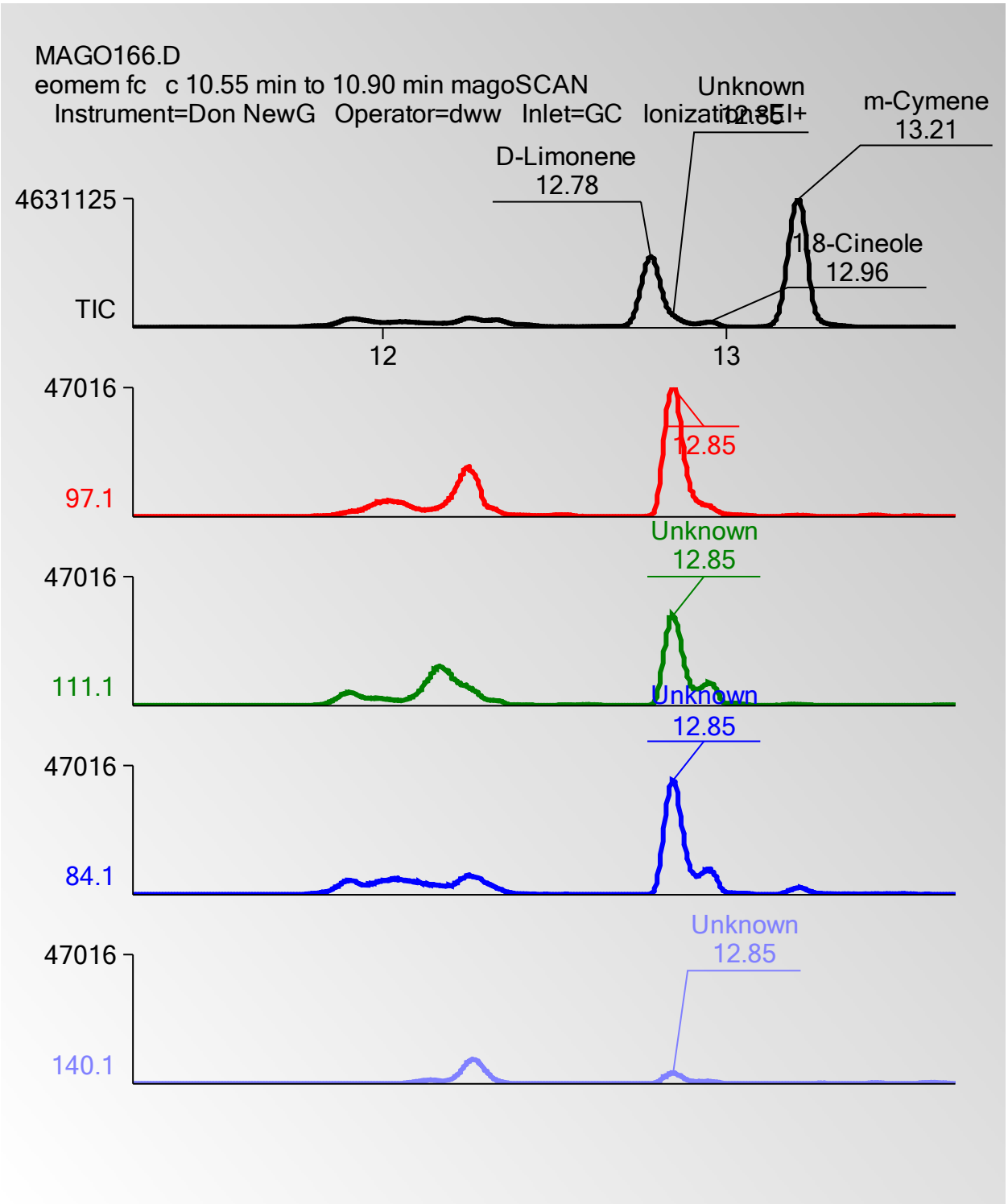


Figure 8 Chromatogram for eomem fc

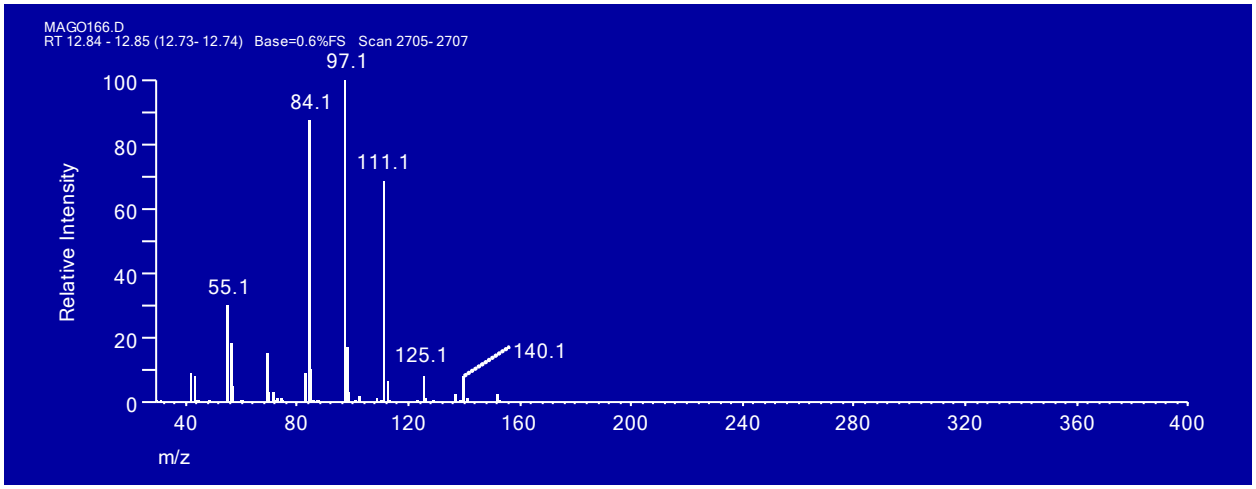


Figure 9 MS of eomem fc at RT 12.84 - 12.85

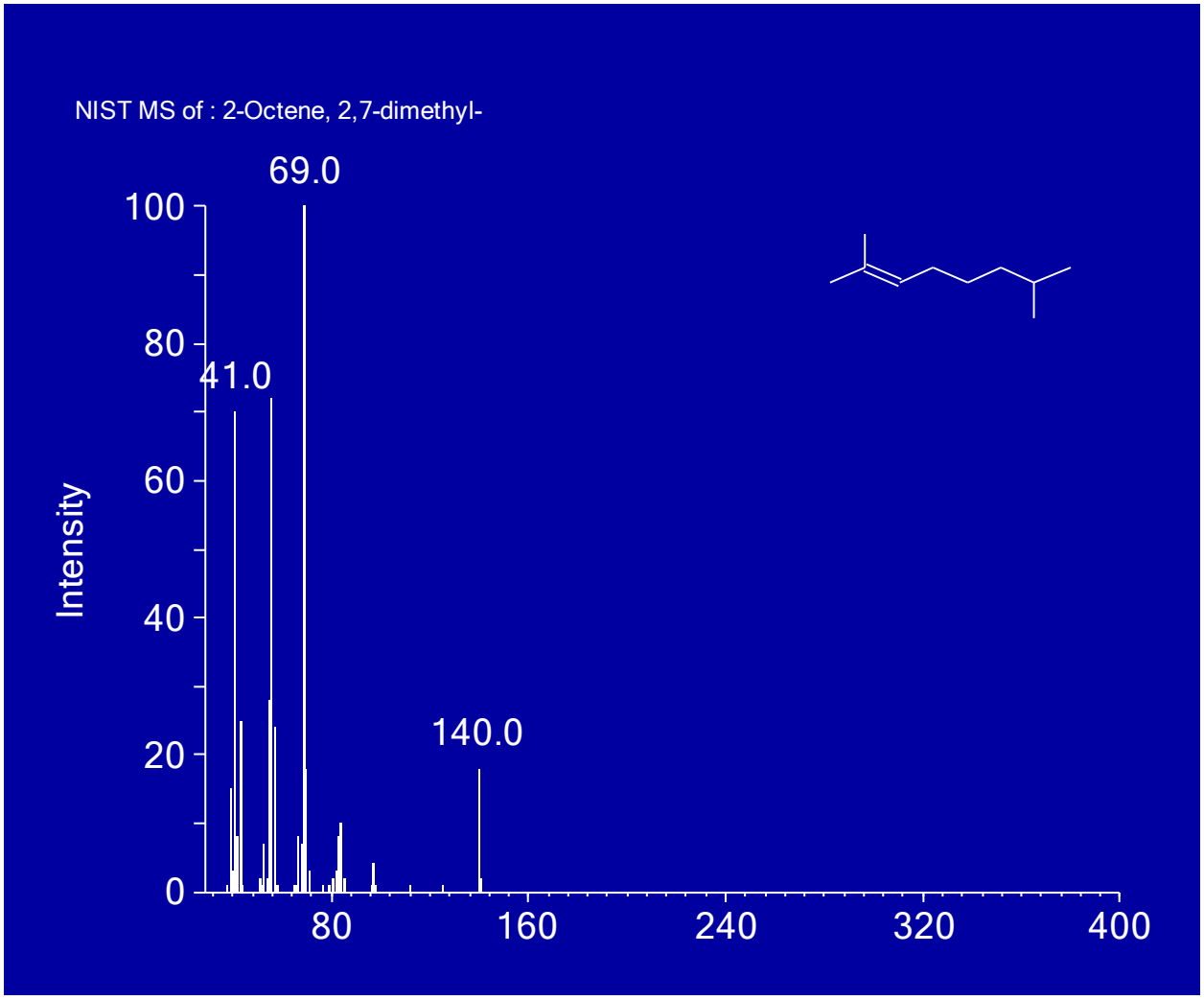


Figure 10 NIST MS of : 2-Octene, 2,7-dimethyl-

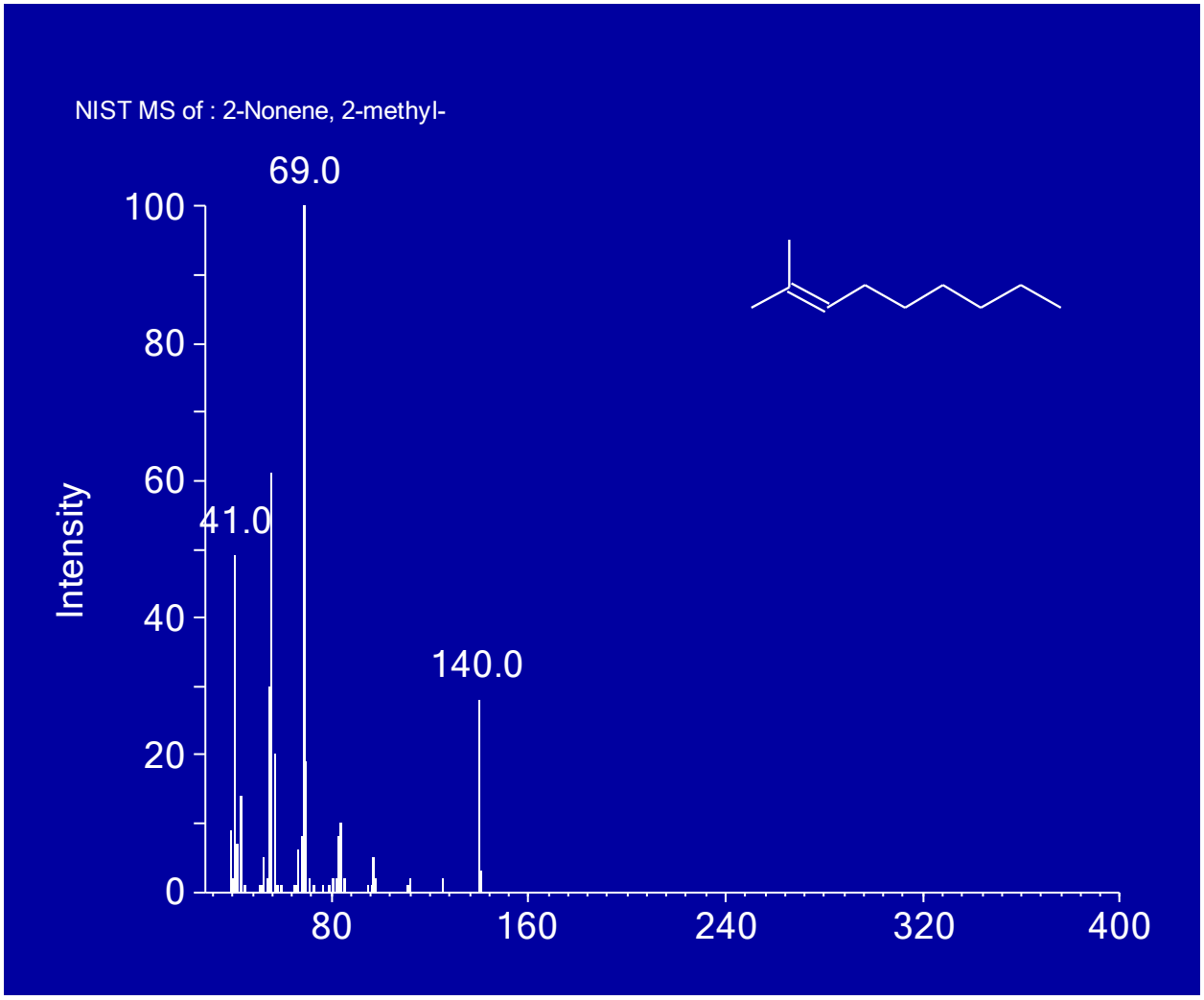


Figure 11 NIST MS of : 2-Nonene, 2-methyl-

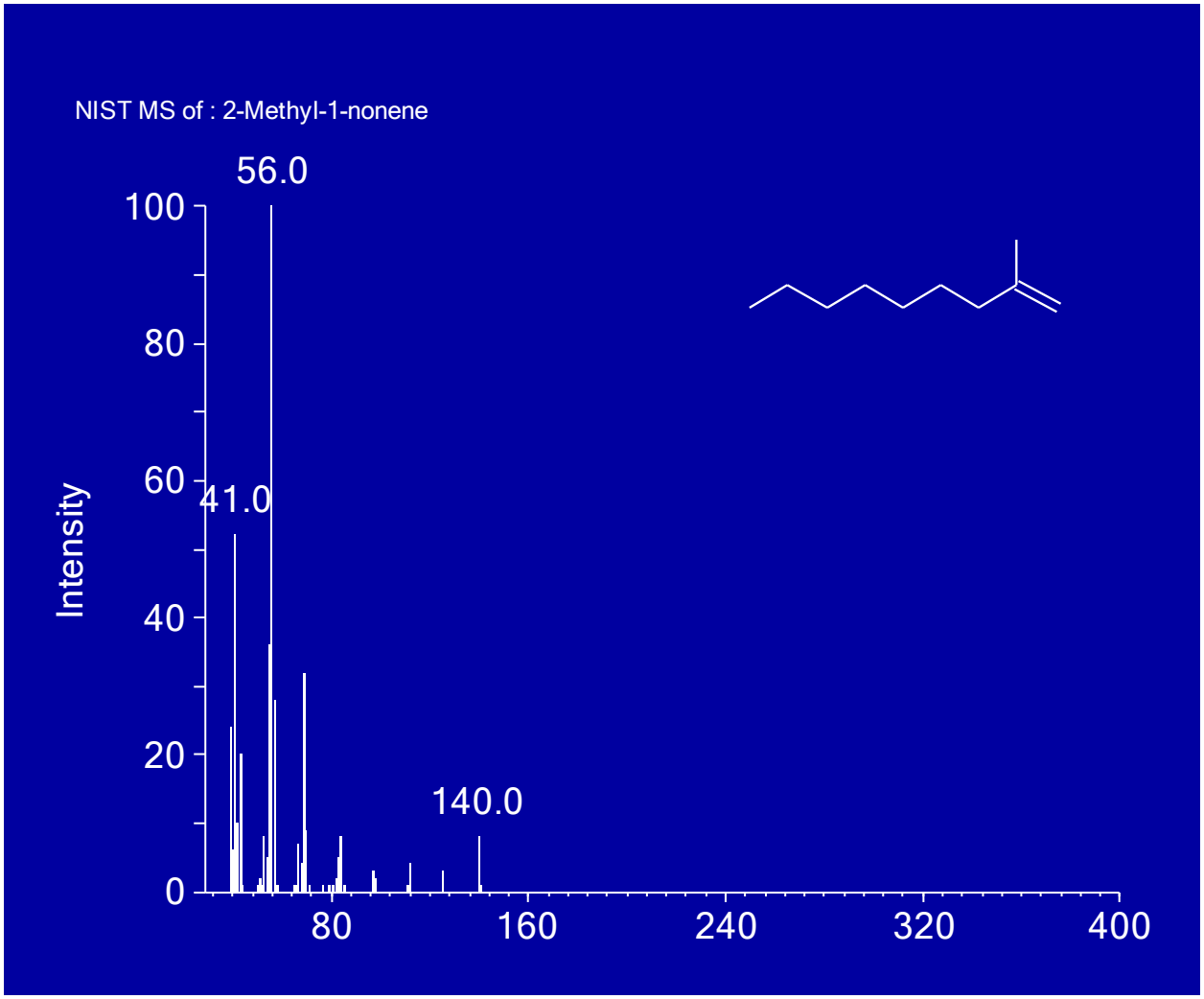


Figure 12 NIST MS of : 2-Methyl-1-nonene

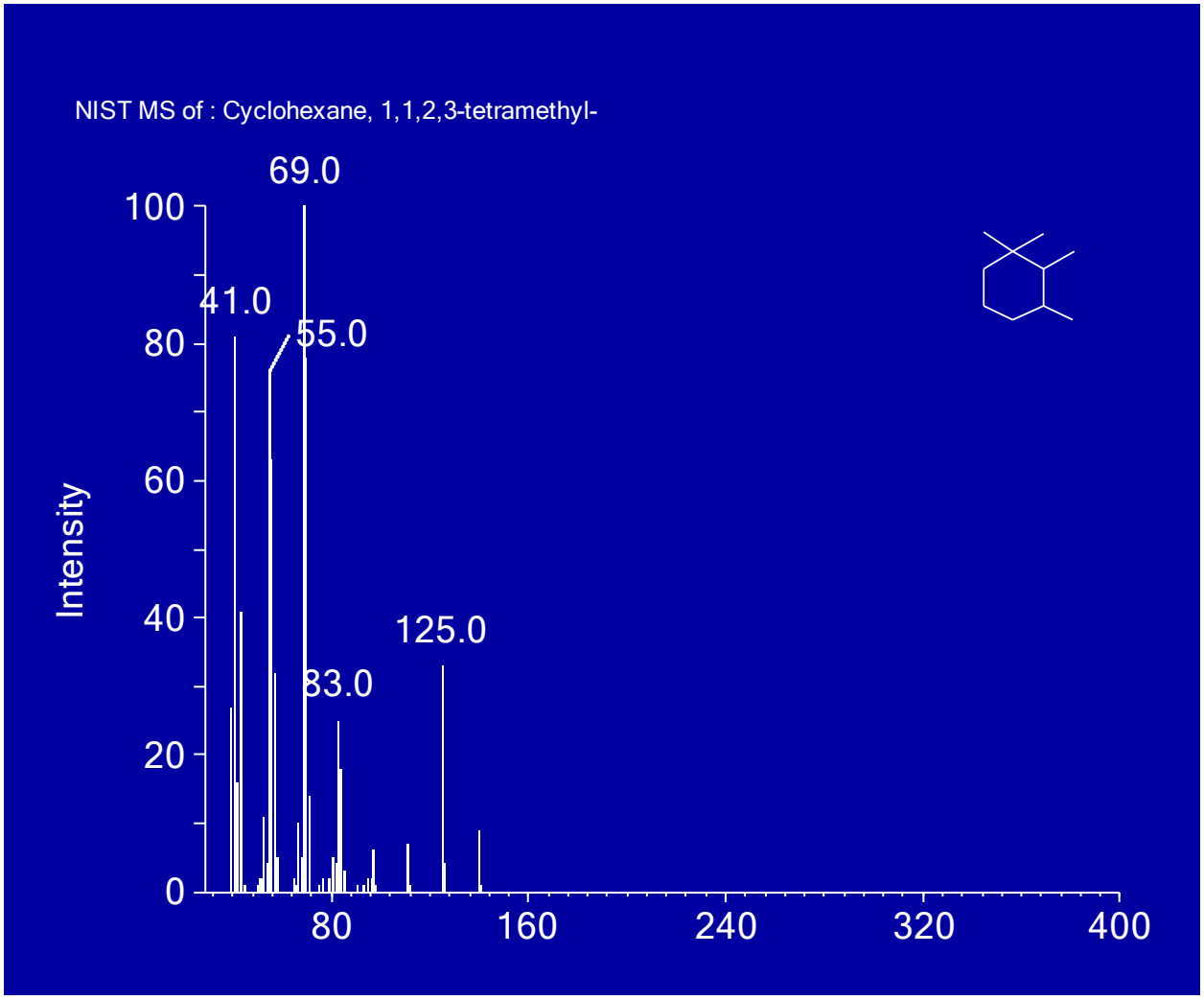


Figure 13 NIST MS of : Cyclohexane, 1,1,2,3-tetramethyl-

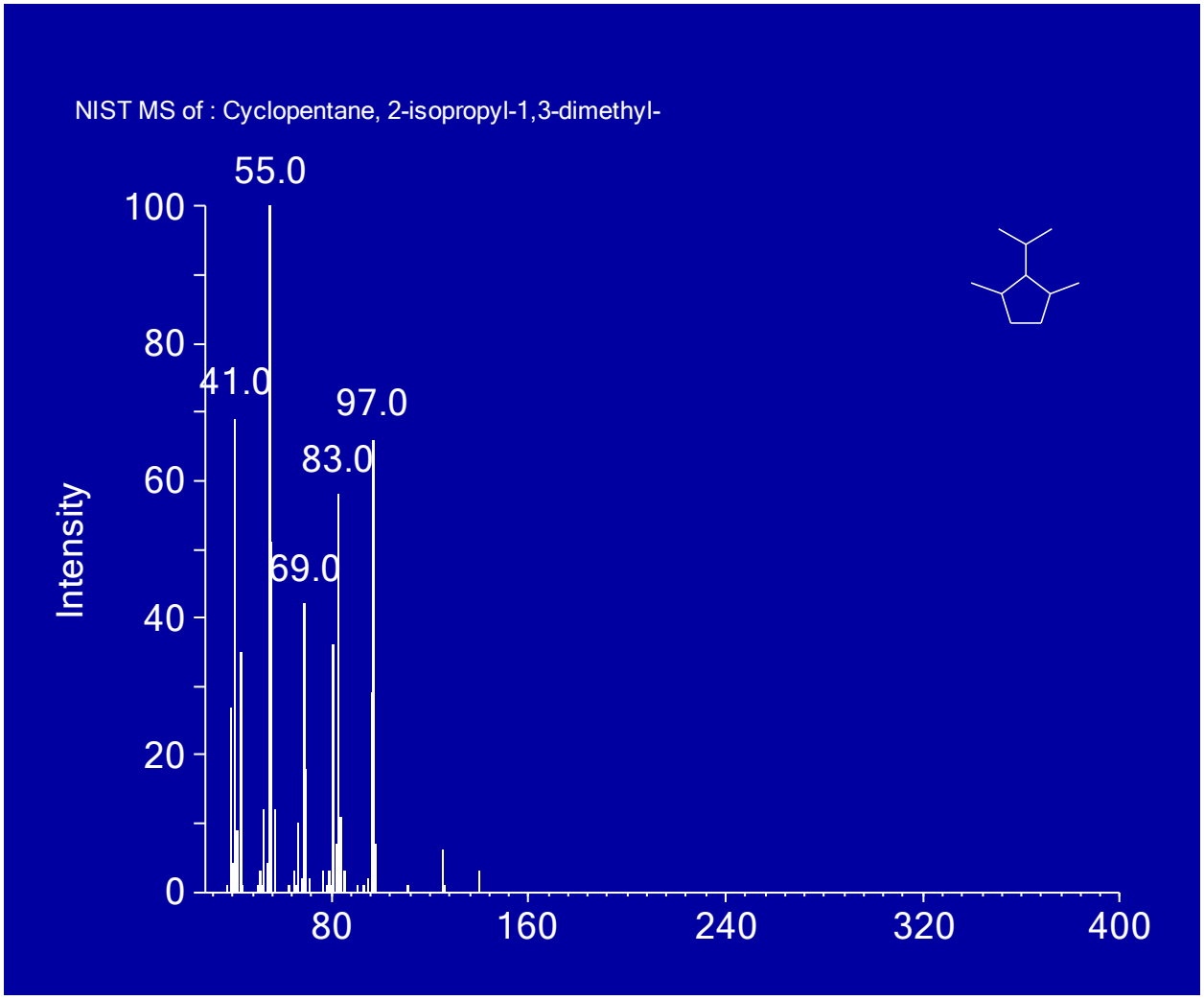


Figure 14 NIST MS of : Cyclopentane, 2-isopropyl-1,3-dimethyl-

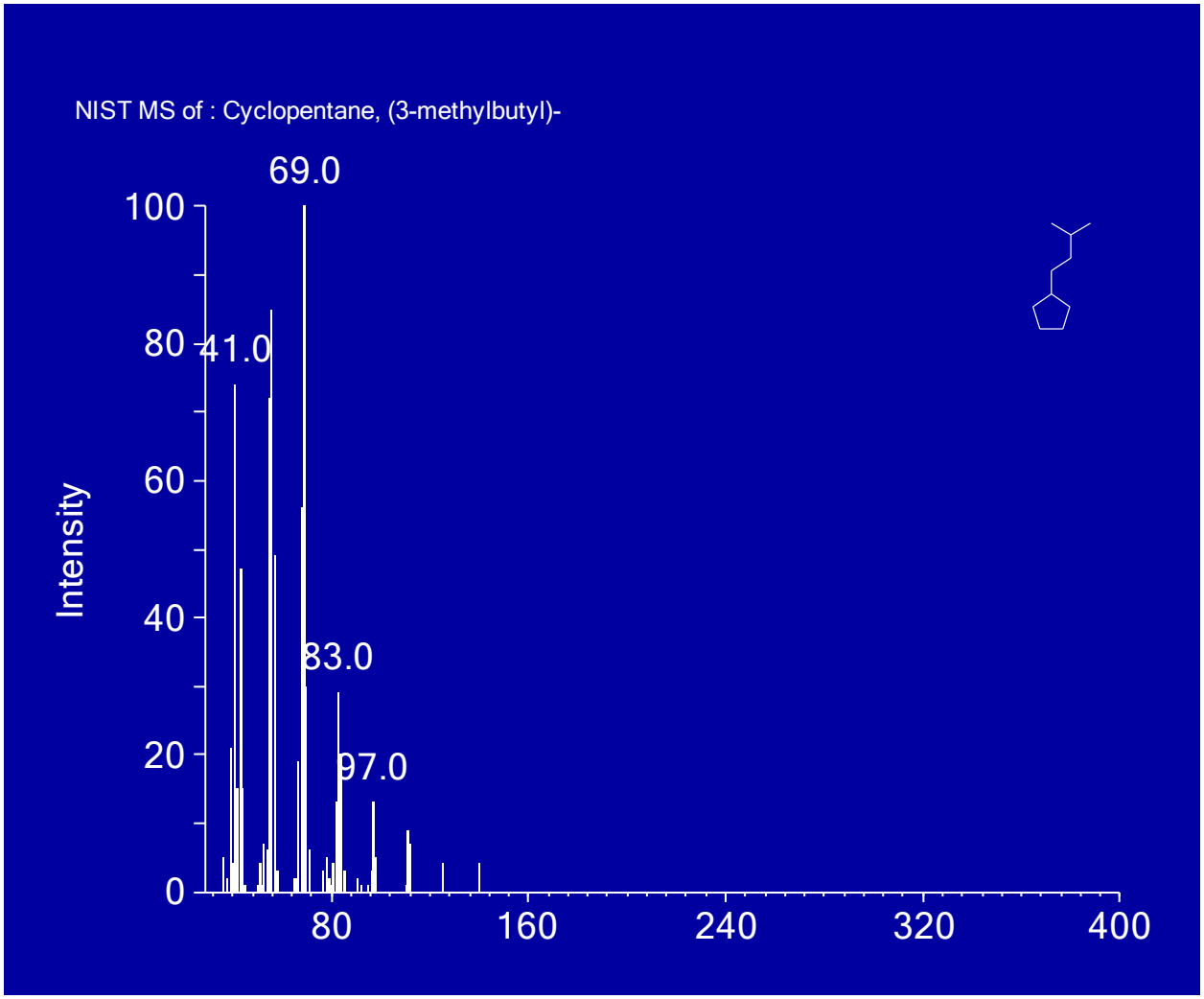


Figure 15 NIST MS of : Cyclopentane, (3-methylbutyl)-

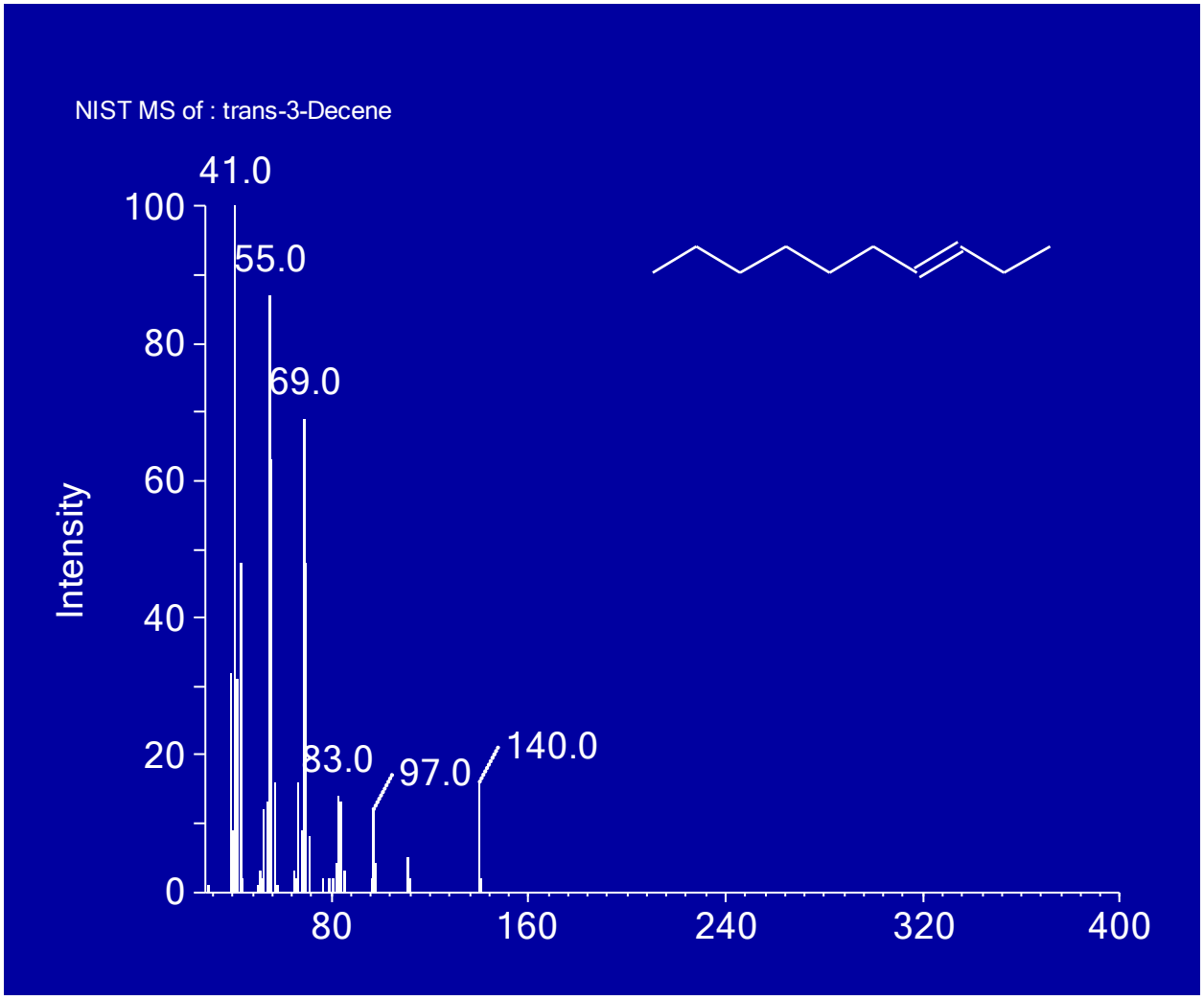


Figure 16 NIST MS of : trans-3-Decene

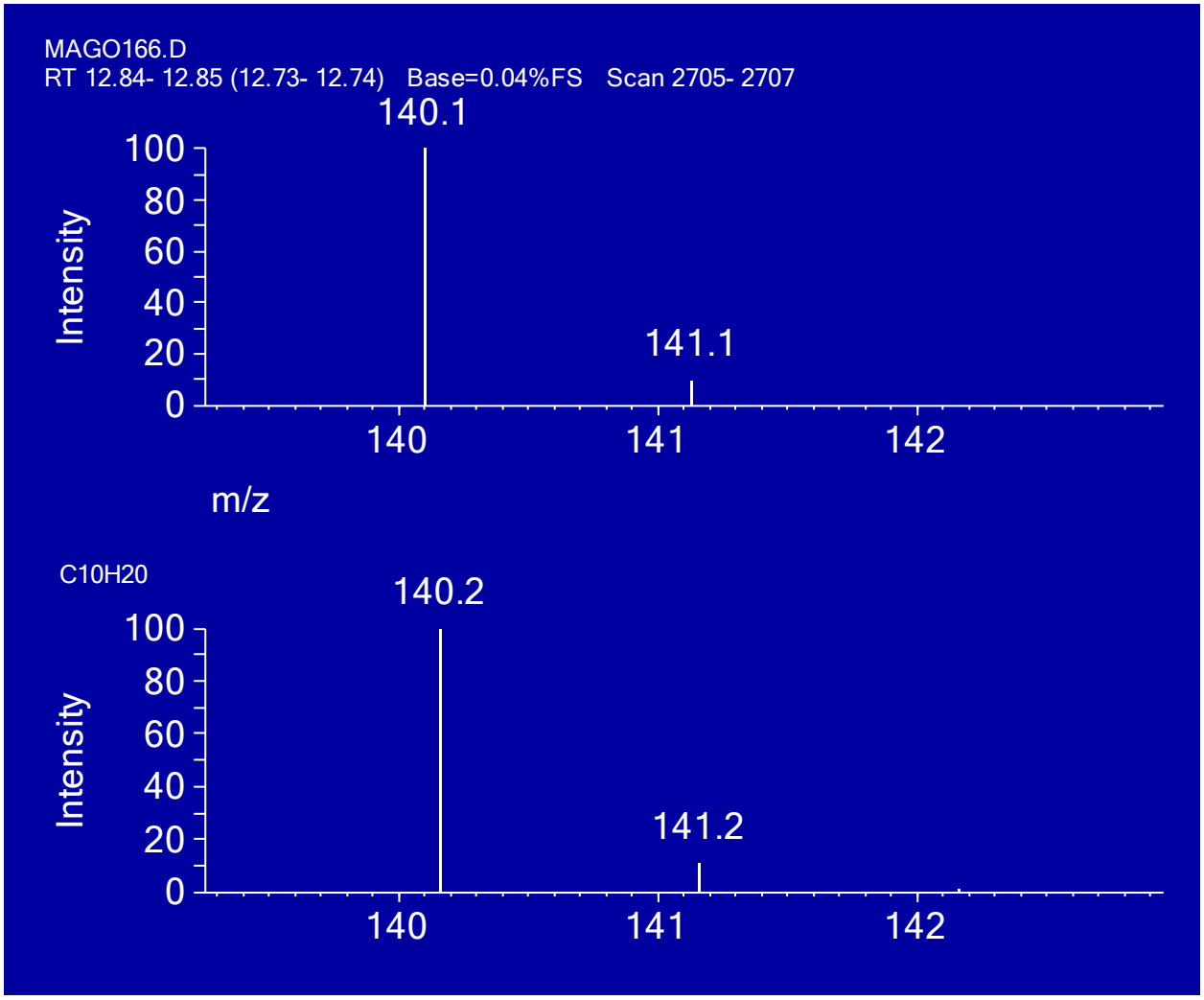


Figure 17 MS of eomem fc at RT 12.84- 12.85 and theoretical isotope peak intensities for $C_{10}H_{20}$.

Table 2 MAGO166.D Scan 2705- 2707 (2679- 2682) Base=0.04%FS RT=12.84- 12.85

Mass	Relative Intensity
140.1	100.0
141.1	9.7

Table 3 theoretical isotope peak intensities for $C_{10}H_{20}$.

Mass	Relative Intensity
140.2	100.0
141.2	11.0
142.2	1.0

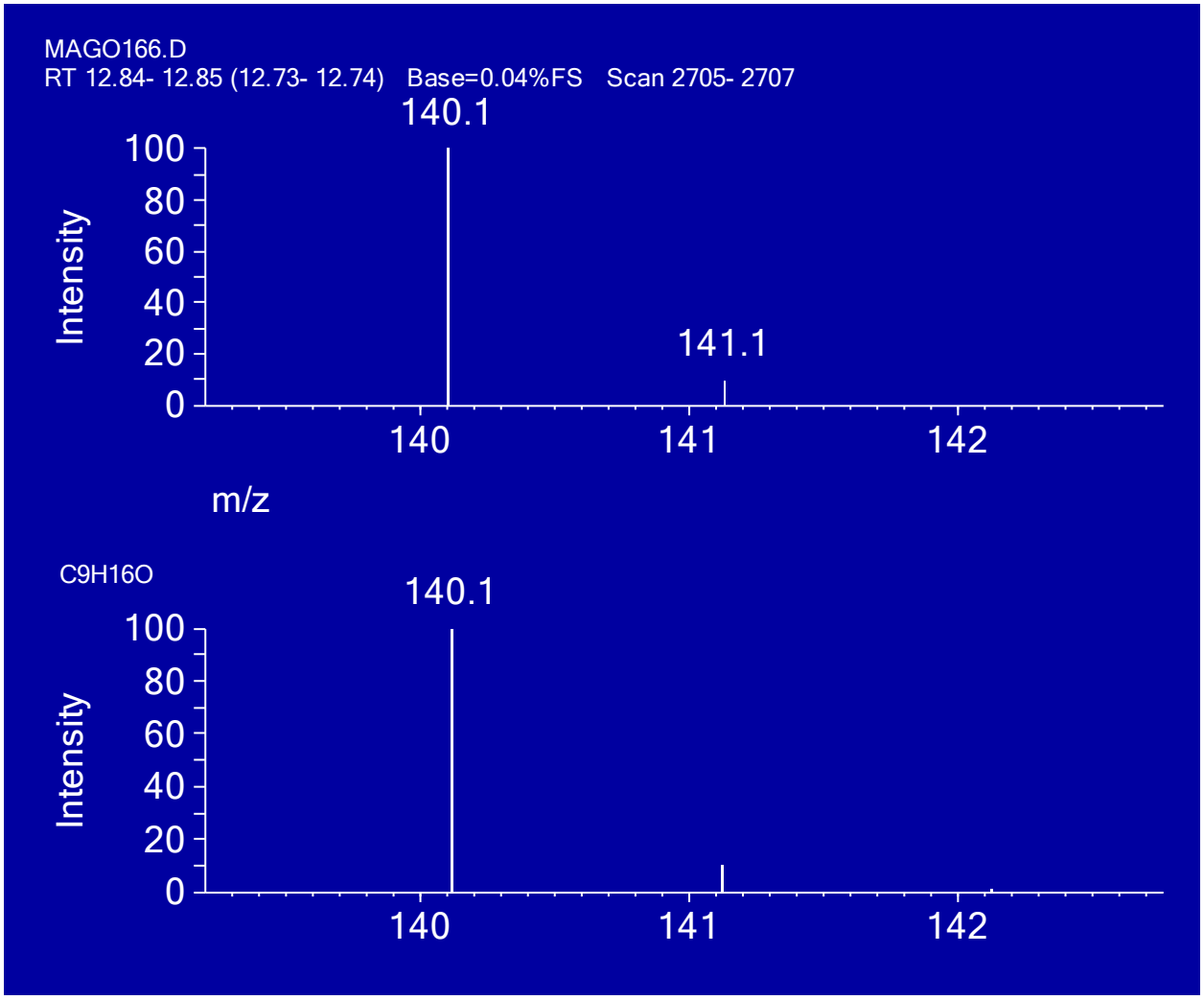


Figure 18 MS of eomem fc at RT 12.84- 12.85 and theoretical isotope peak intensities for $C_9H_{16}O$.

Table 4 MAGO166.D Scan 2705- 2707 (2679- 2682) Base=0.04%FS RT=12.84- 12.85

Mass	Relative Intensity
140.1	100.0
141.1	9.7

Table 5 theoretical isotope peak intensities for $C_9H_{16}O$

Mass	Relative Intensity
140.1	100.0
141.1	10.0
142.1	1.0

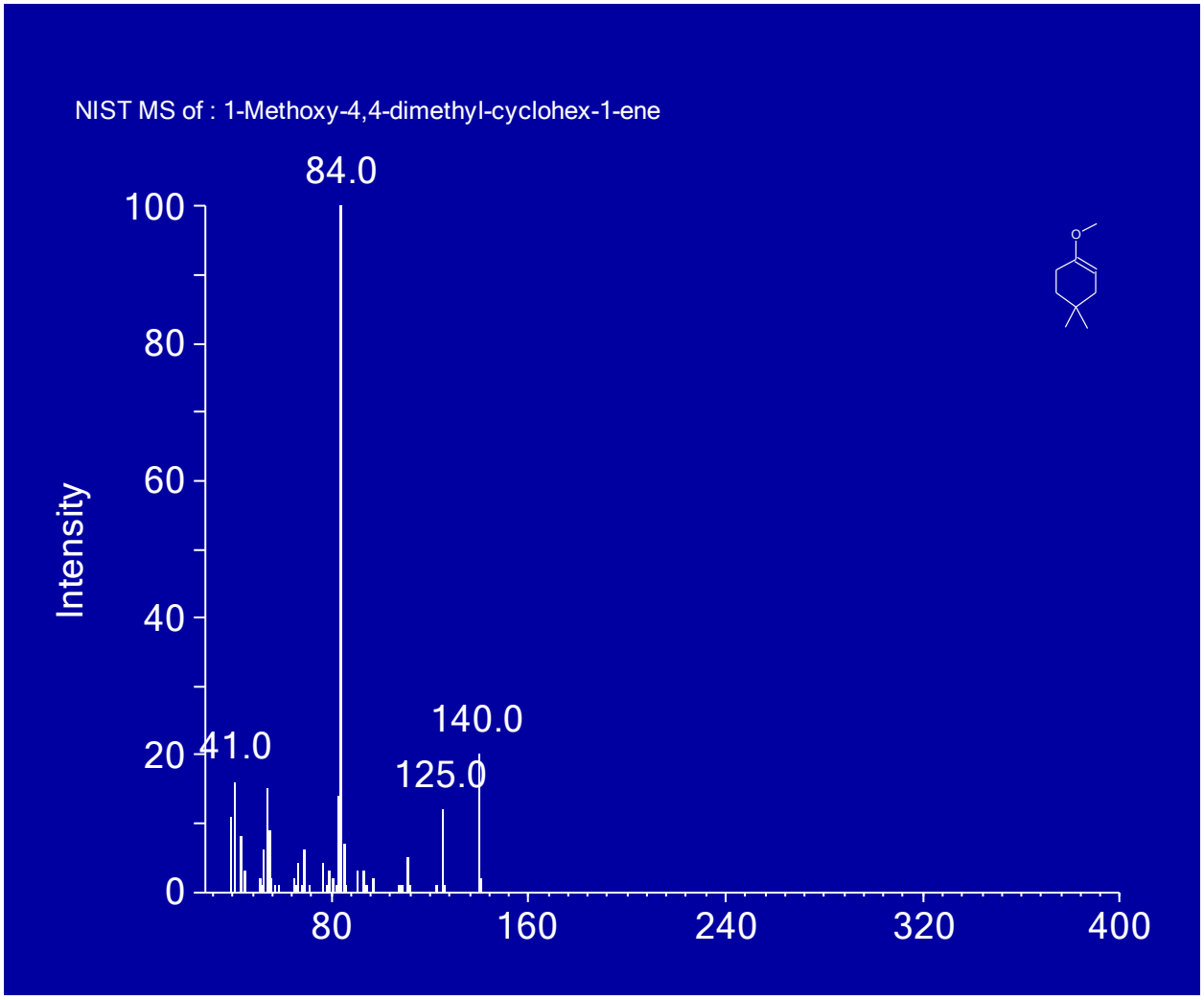


Figure 19 NIST MS of : 1-Methoxy-4,4-dimethyl-cyclohex-1-ene

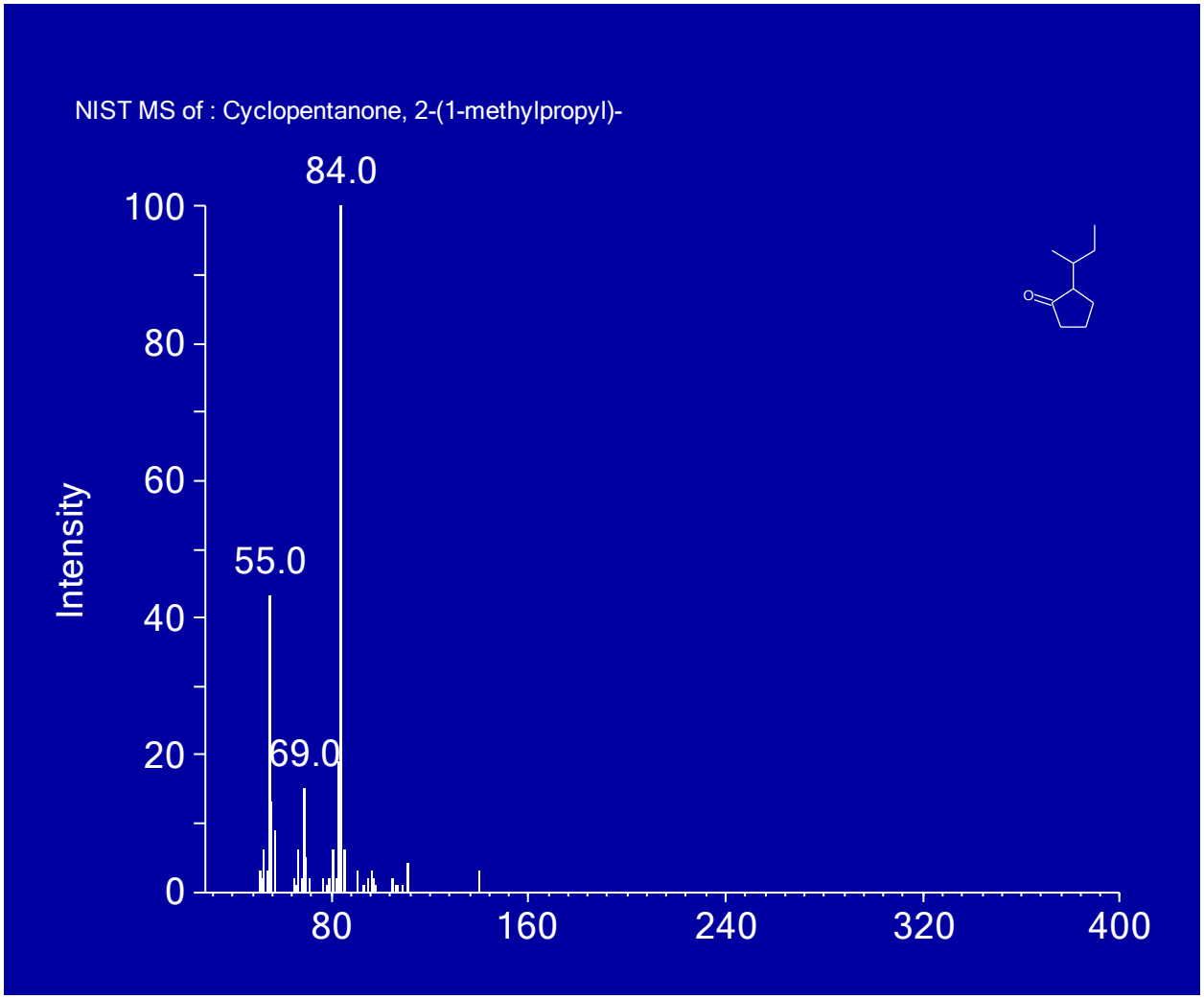


Figure 20 NIST MS of : Cyclopentanone, 2-(1-methylpropyl)-

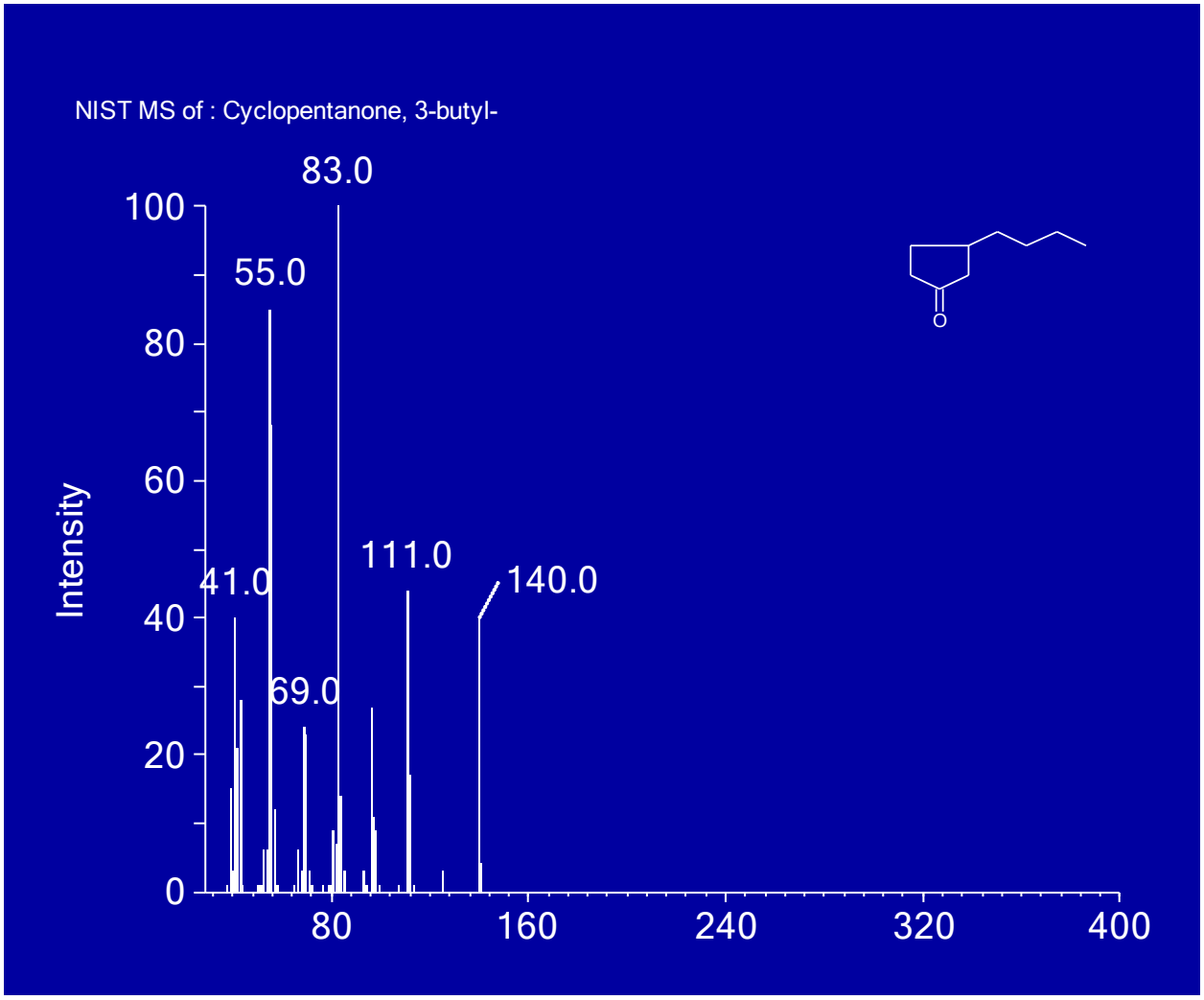


Figure 21 NIST MS of : Cyclopentanone, 3-butyl-

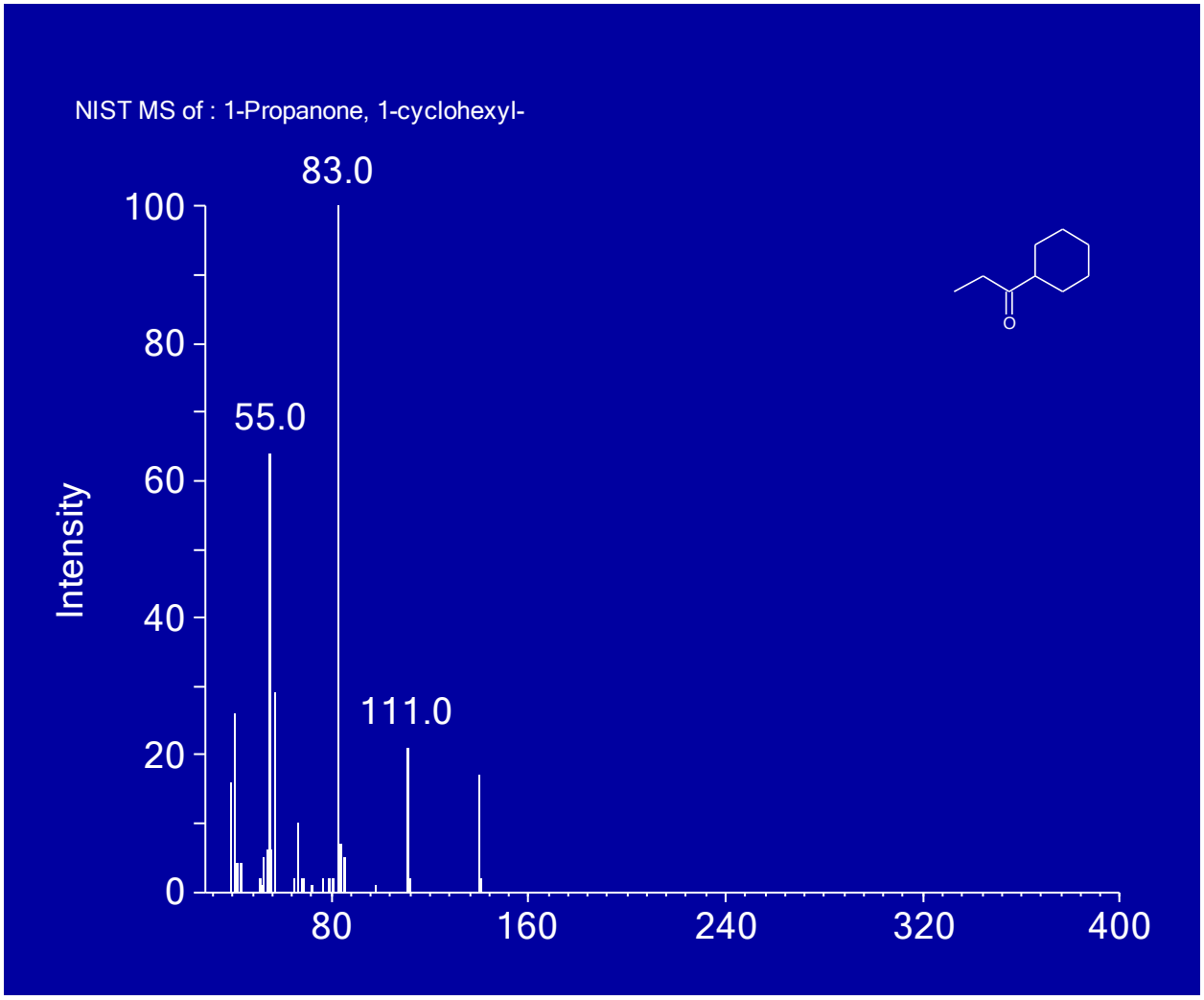


Figure 22 NIST MS of : 1-Propanone, 1-cyclohexyl-

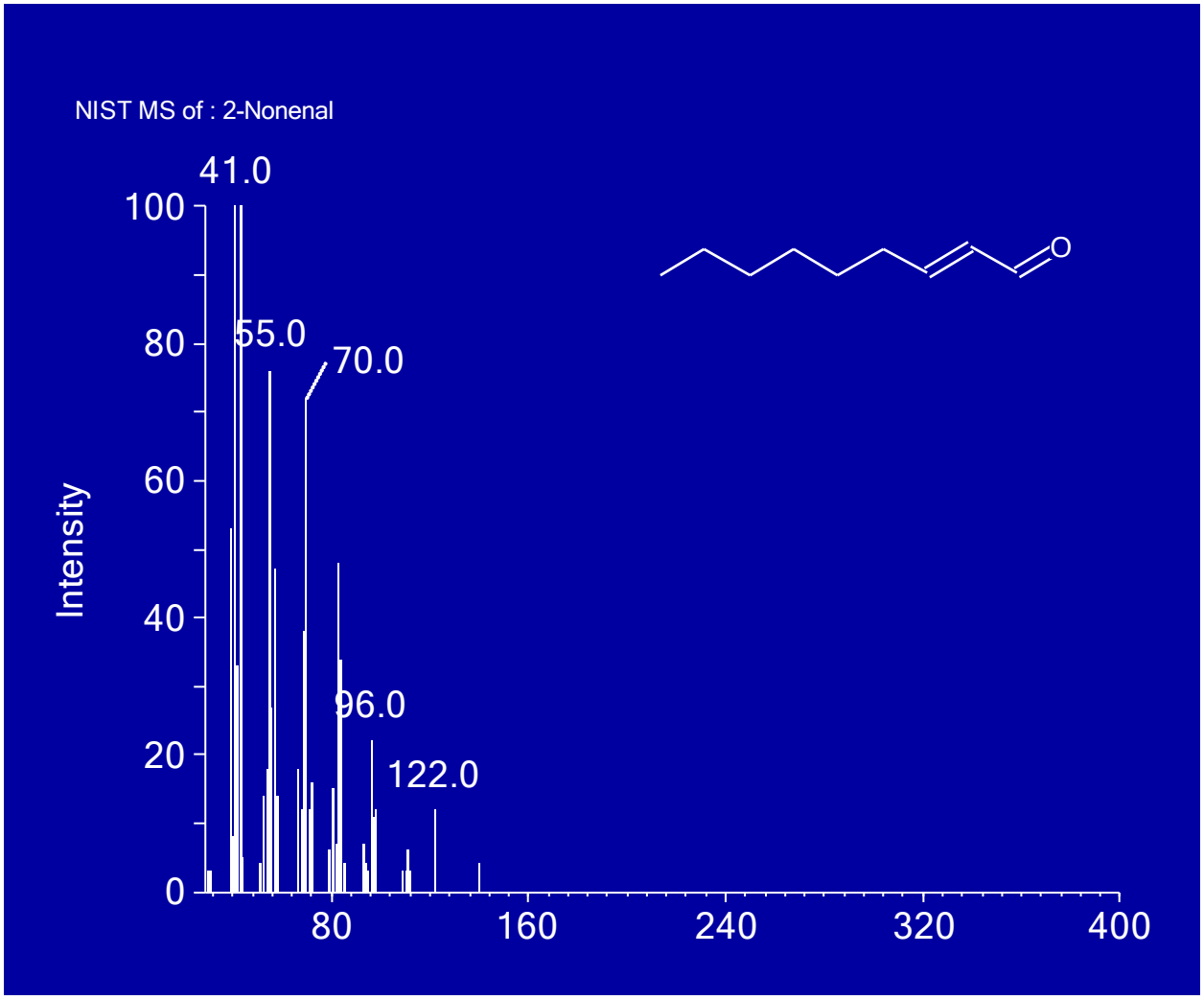


Figure 23 NIST MS of : 2-Nonenal

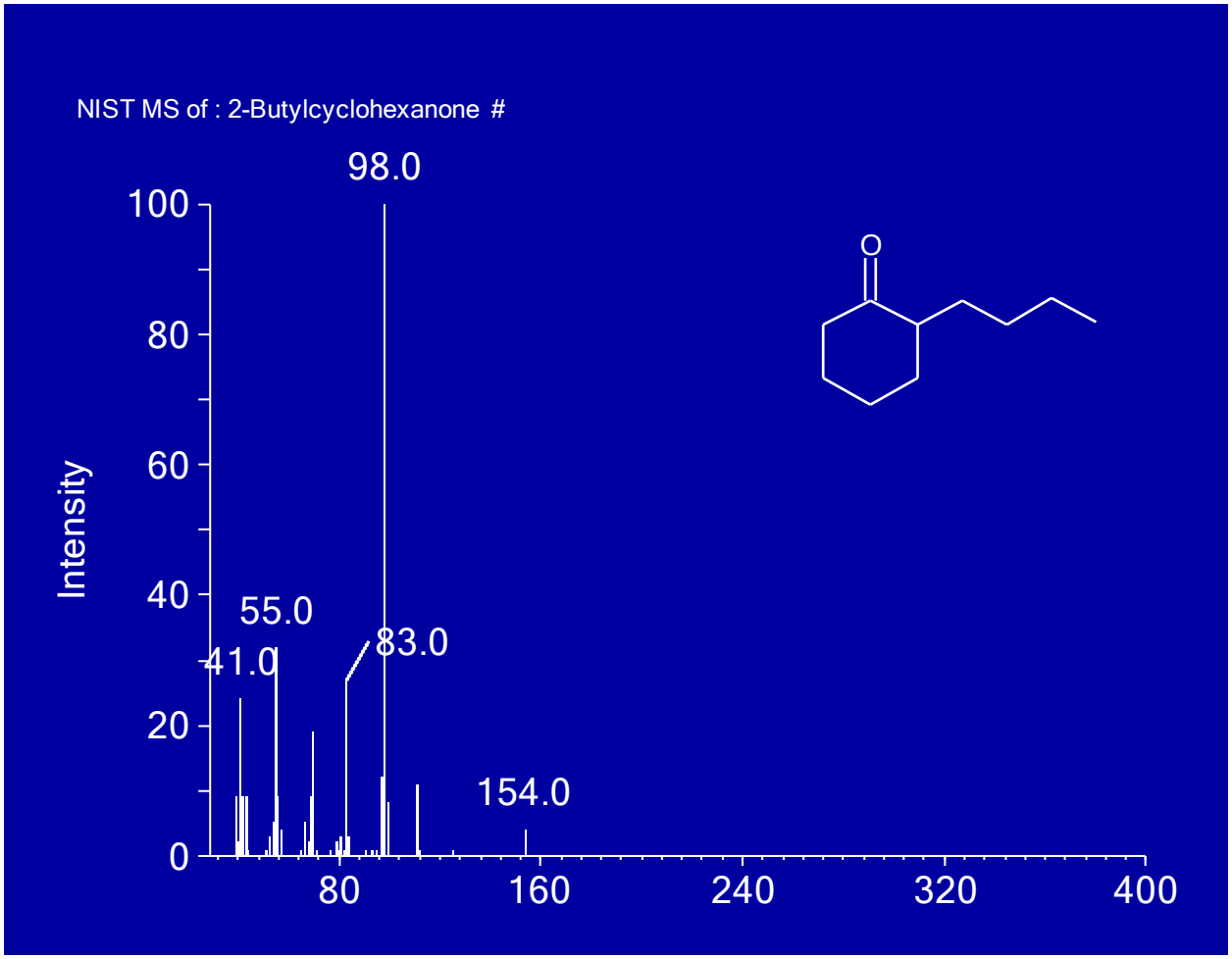


Figure 24 NIST MS of : 2-Butylcyclohexanone #

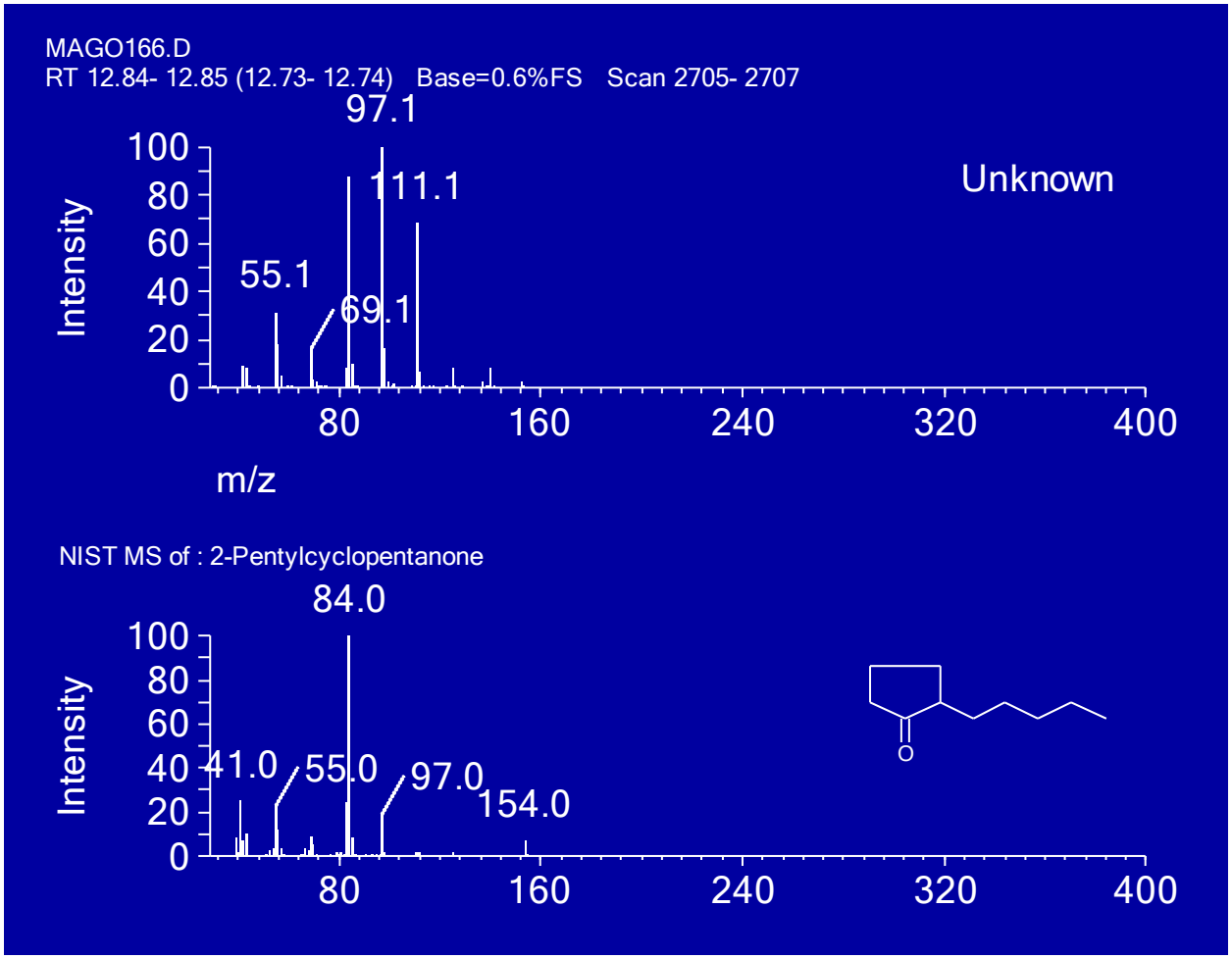


Figure 25 MS of eomem fc at RT 12.84- 12.85 and NIST MS of : 2-Pentylcyclopentanone Match factor 59.5