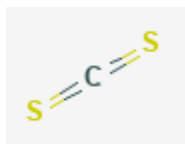


# Supplementary data S1. Compound fragmentation spectra with corresponding library matches (where available) and GC-MS chromatograms.

For number coding and references please see Table 2.

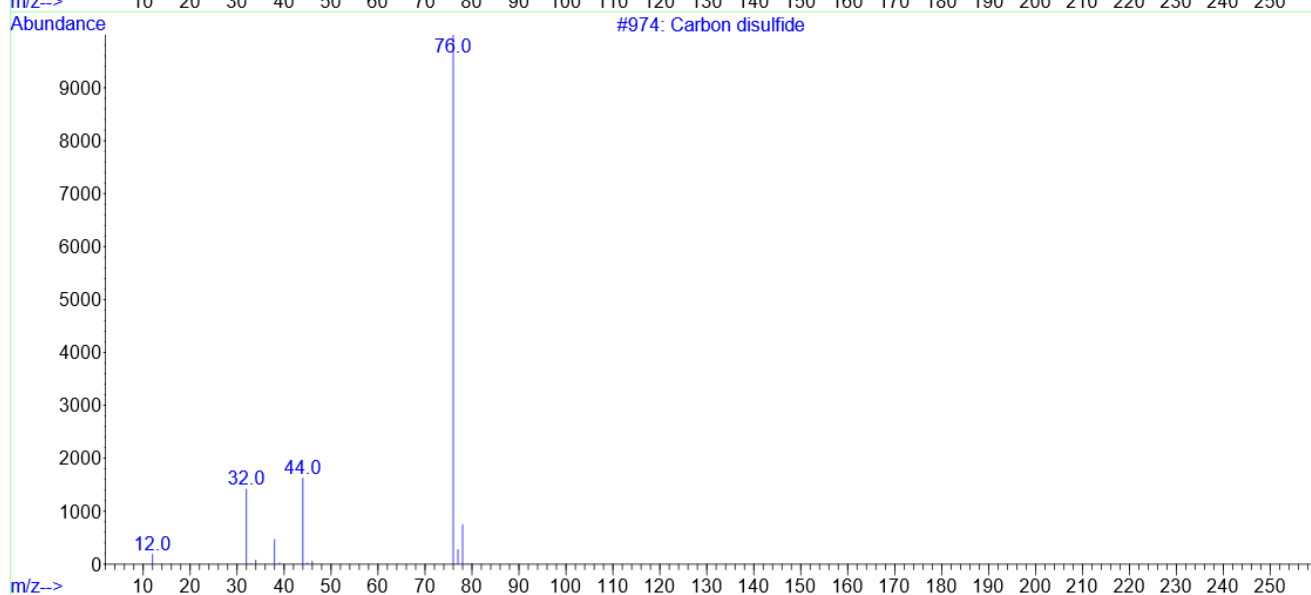
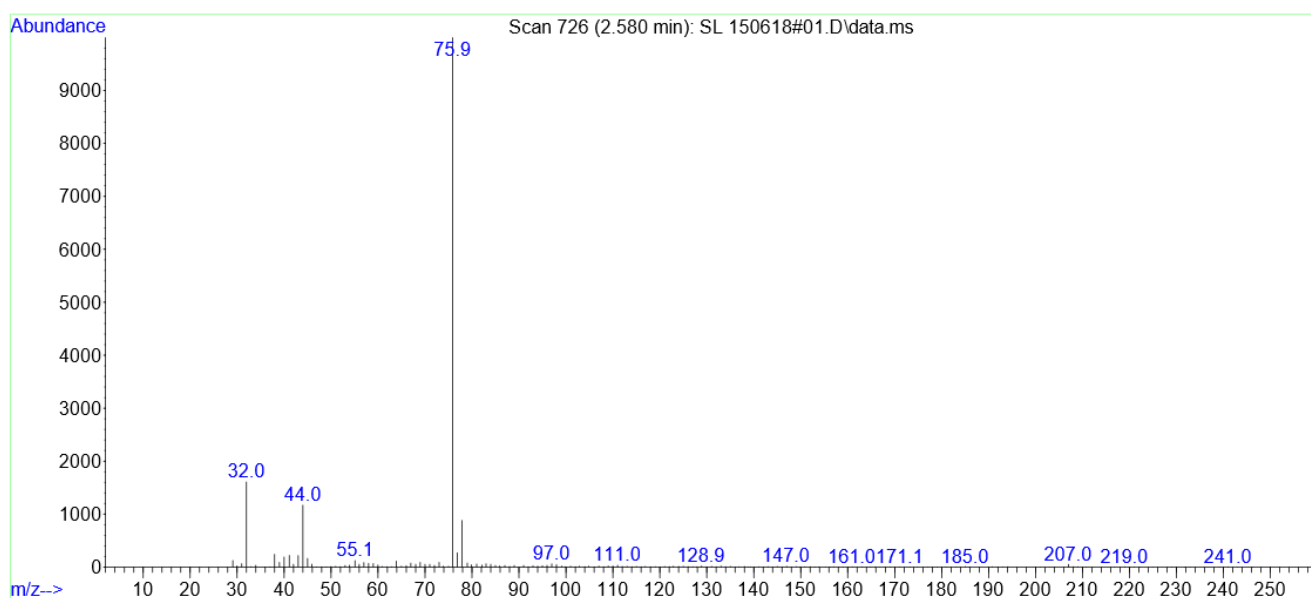
## 1. Carbon disulfide



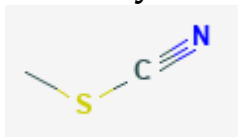
Library Searched : C:\Database\NIST11.L

Quality : 90

ID : Carbon disulfide



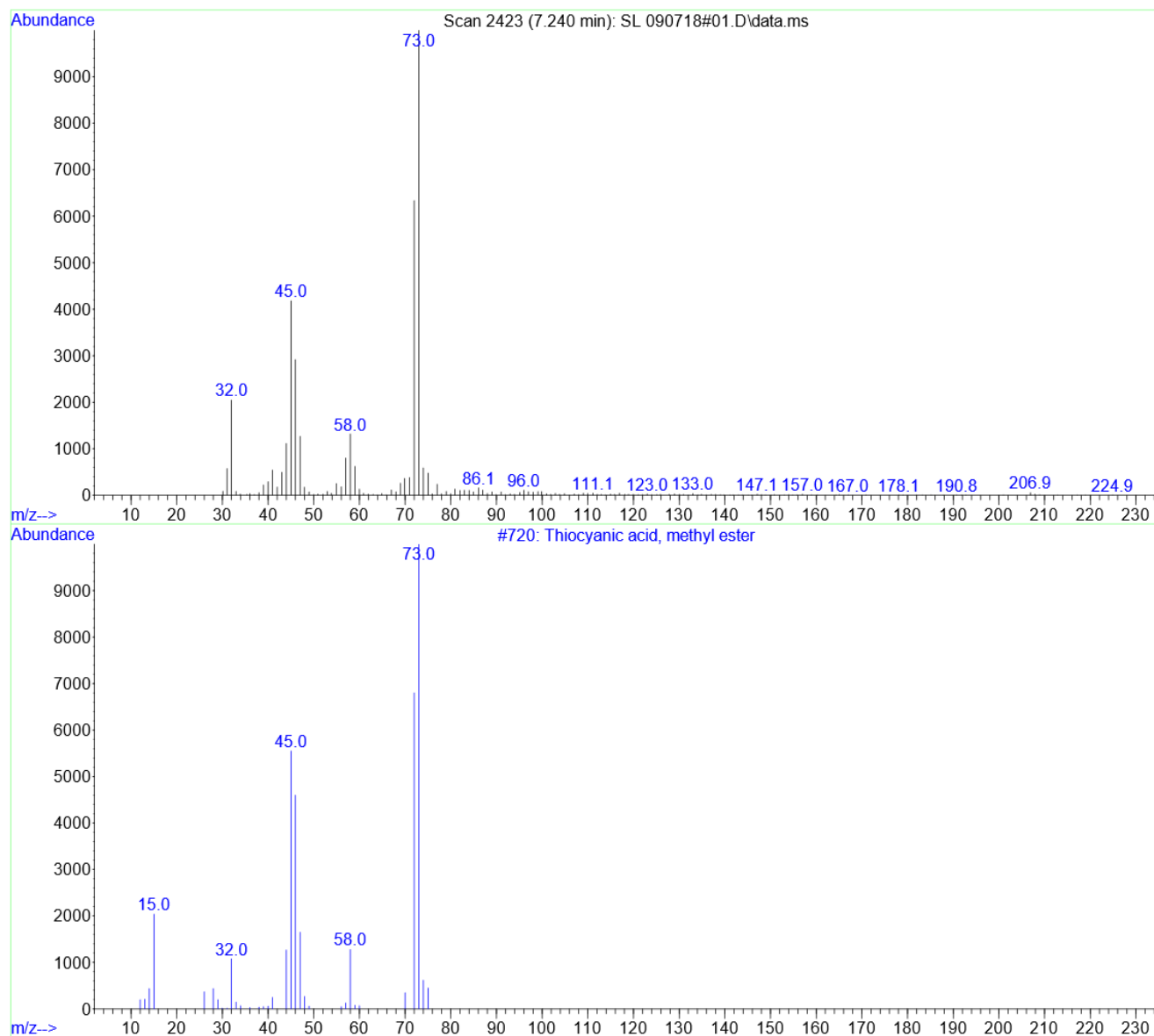
## 2. Methyl thiocyanate



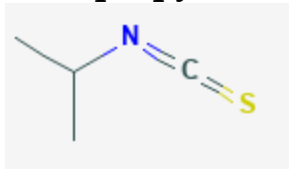
Library Searched : C:\Database\NIST11.L

Quality : 91

ID : Thiocyanic acid, methyl ester



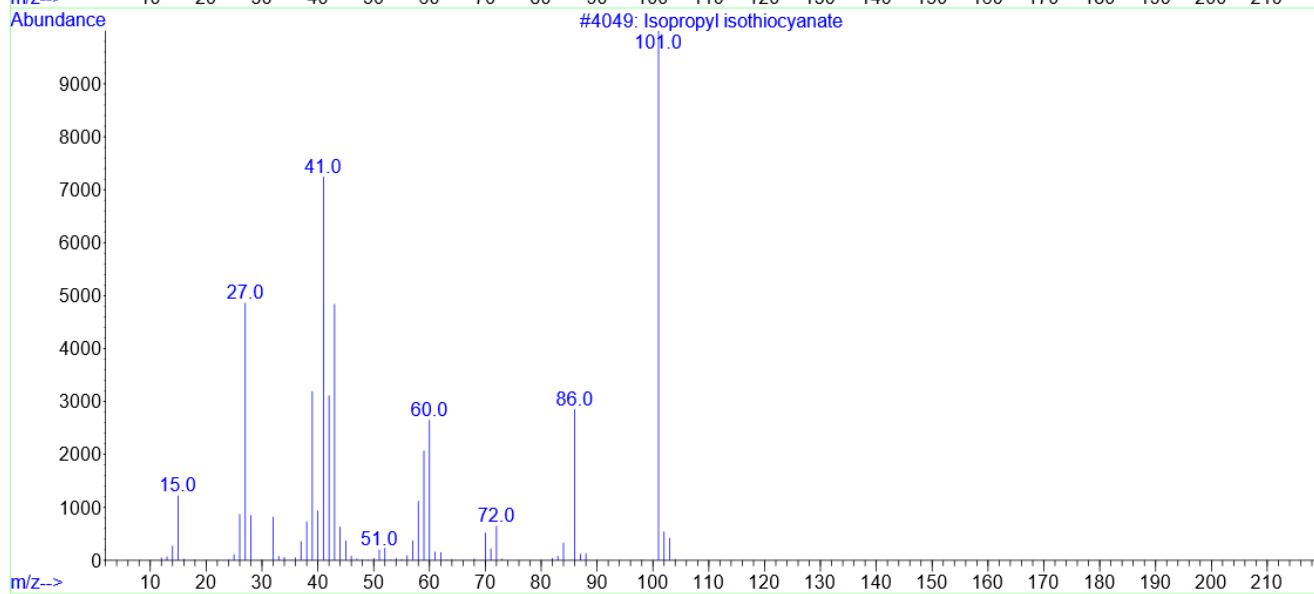
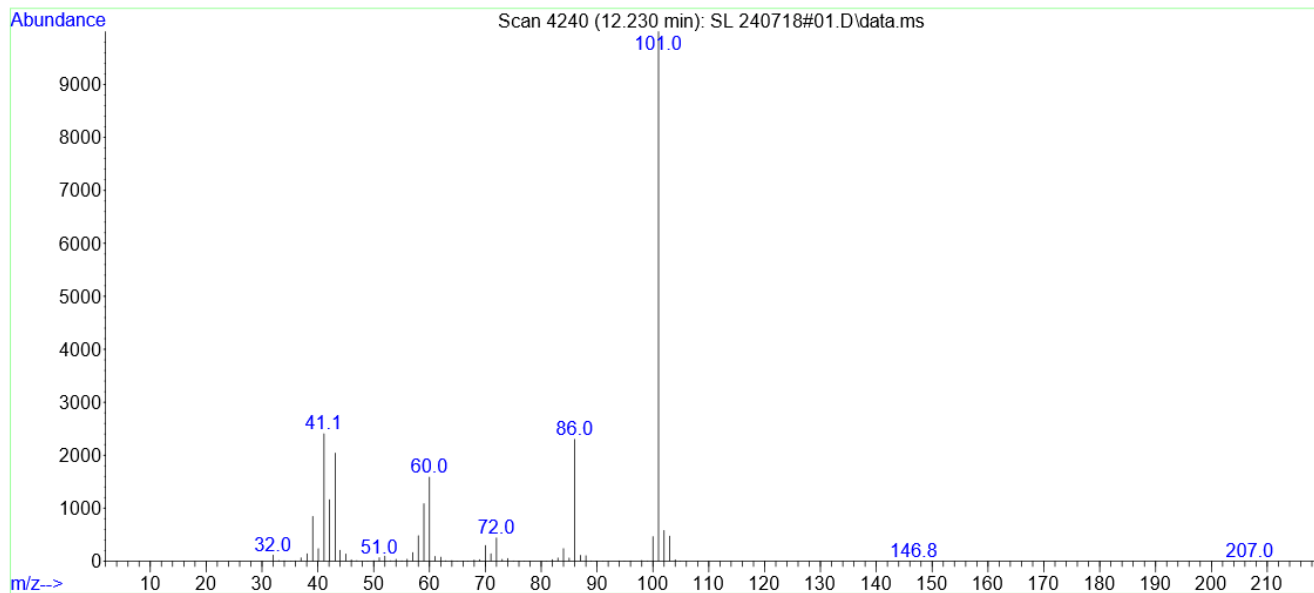
### 3. Isopropyl isothiocyanate



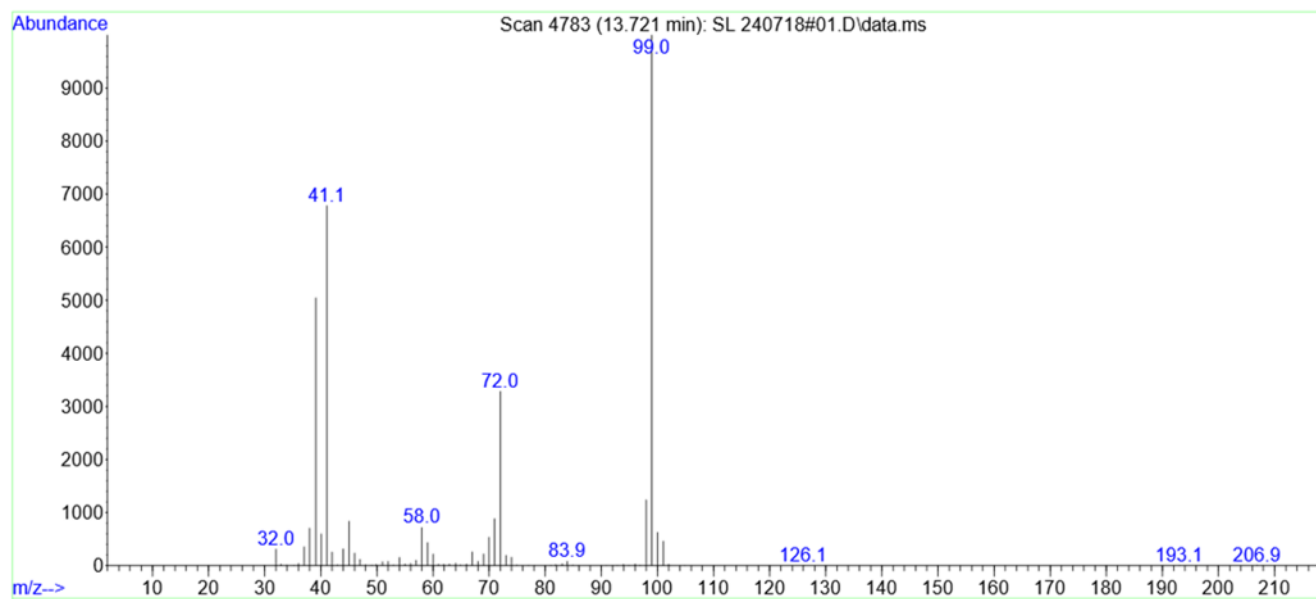
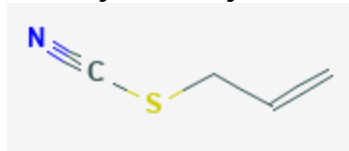
Library Searched : C:\Database\NIST11.L

Quality : 91

ID : Isopropyl isothiocyanate

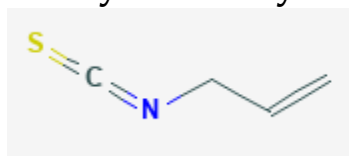


#### 4. Allyl thiocyanate





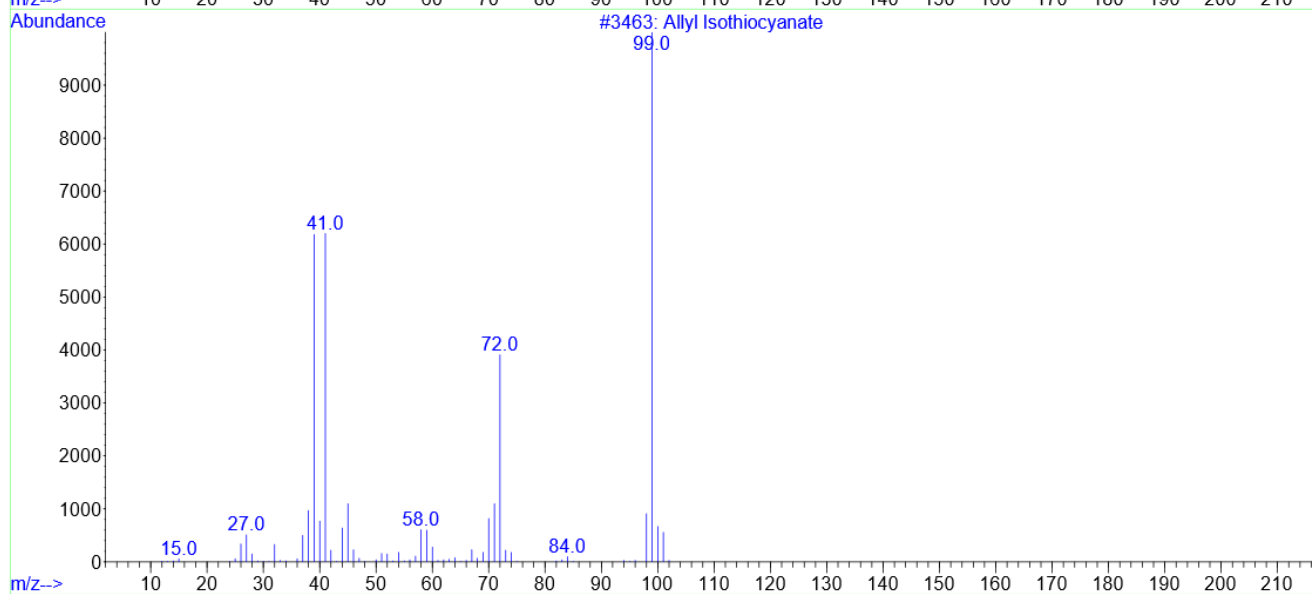
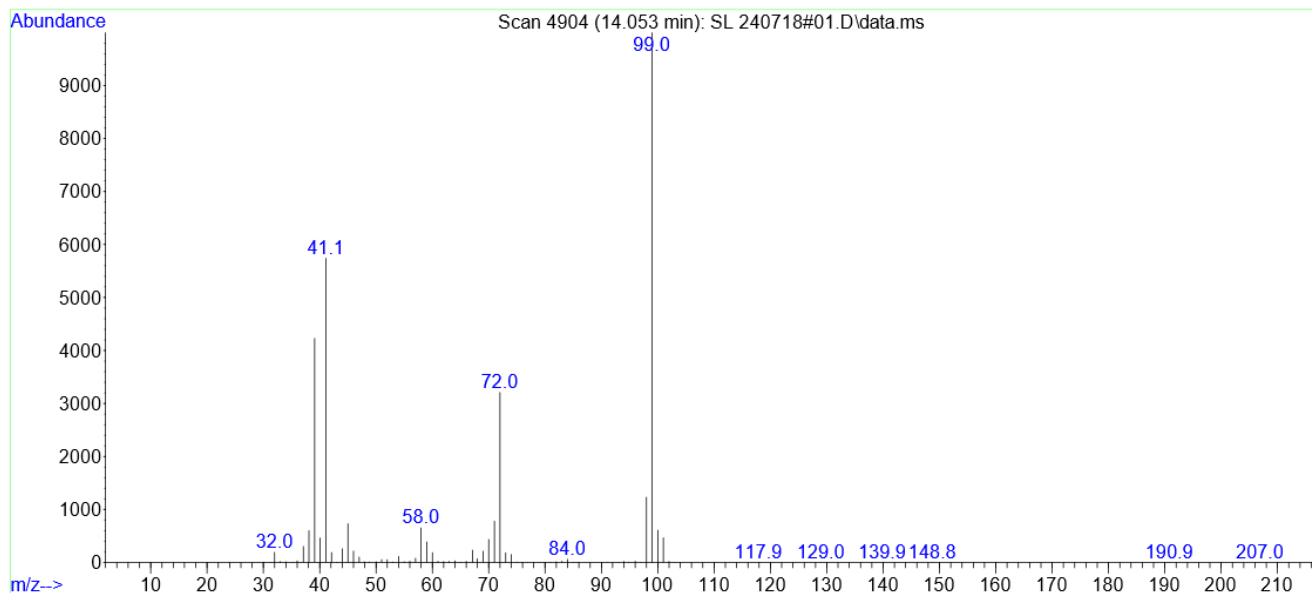
## 5. Allyl isothiocyanate (peak 1)



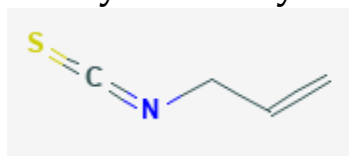
Library Searched : C:\Database\NIST11.L

Quality : 91

ID : Allyl Isothiocyanate



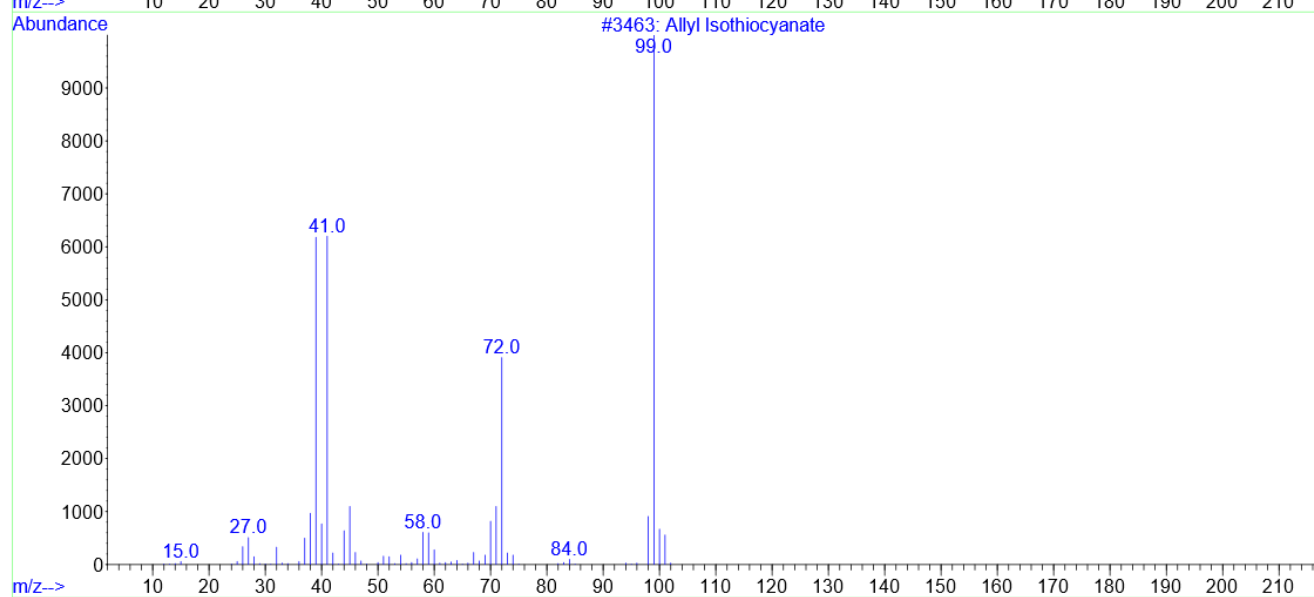
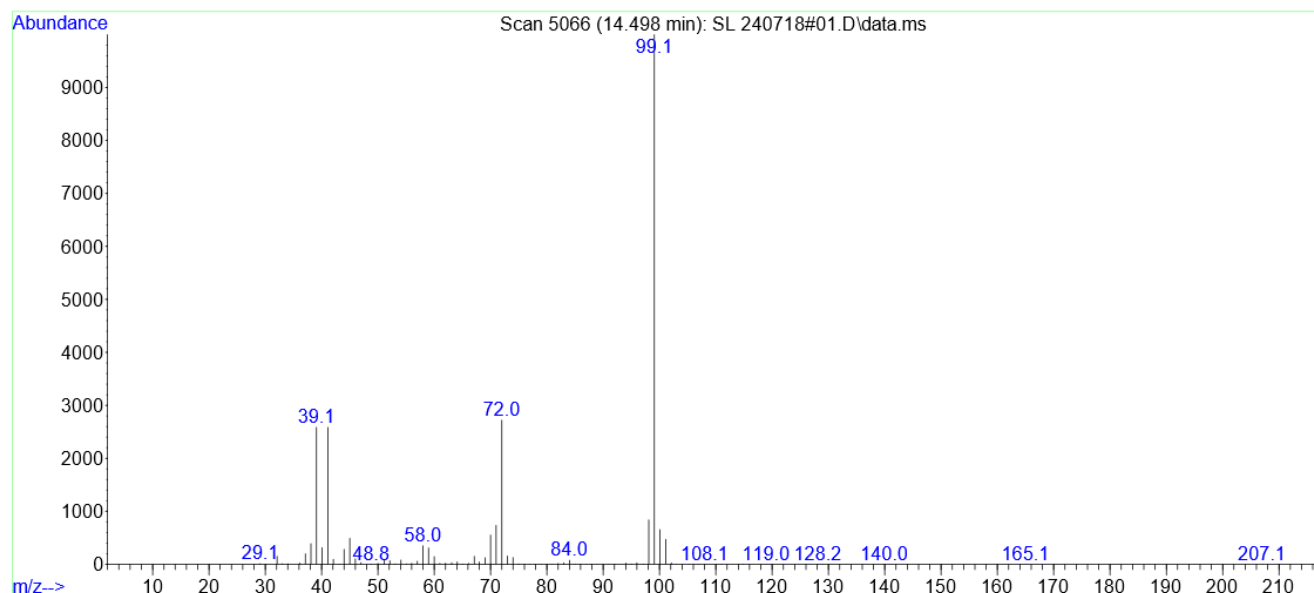
## 6. Allyl isothiocyanate (peak 2)



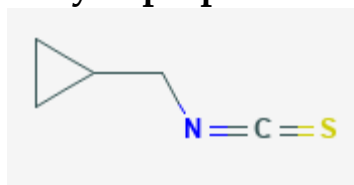
Library Searched : C:\Database\NIST11.L

Quality : 94

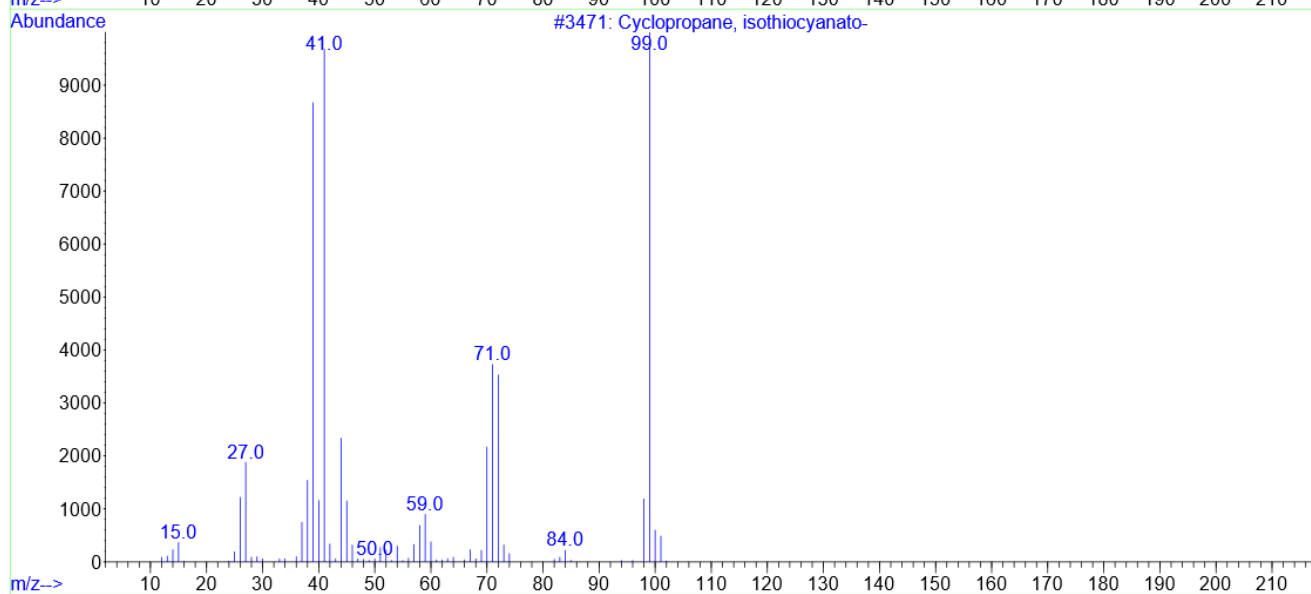
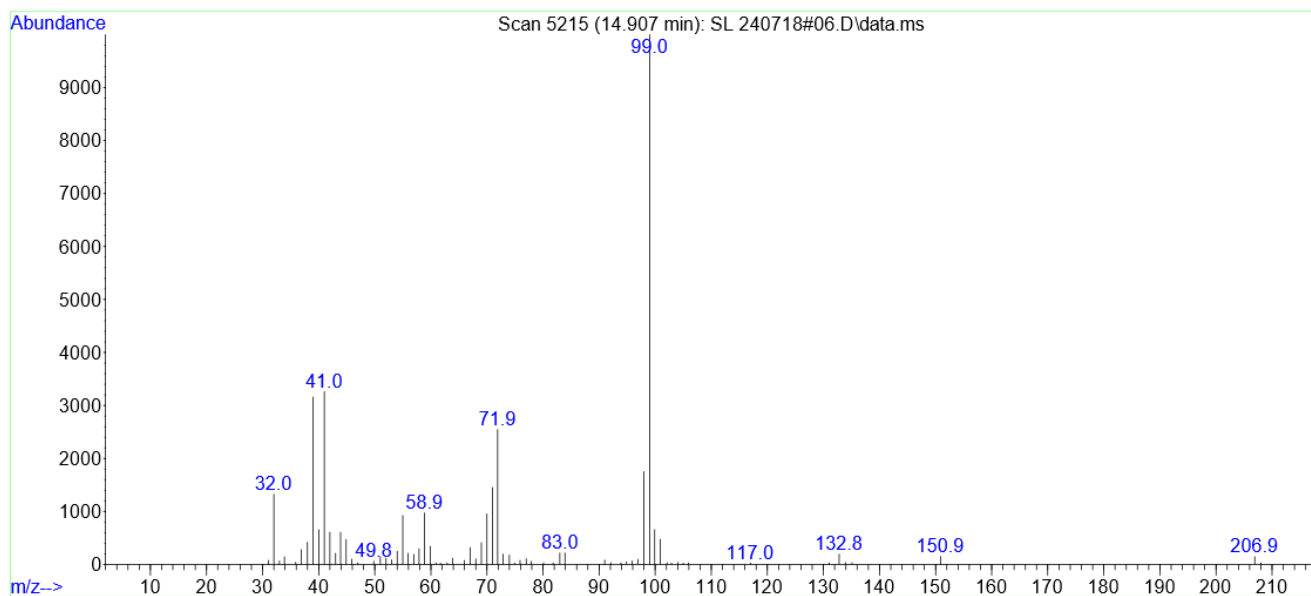
ID : Allyl Isothiocyanate



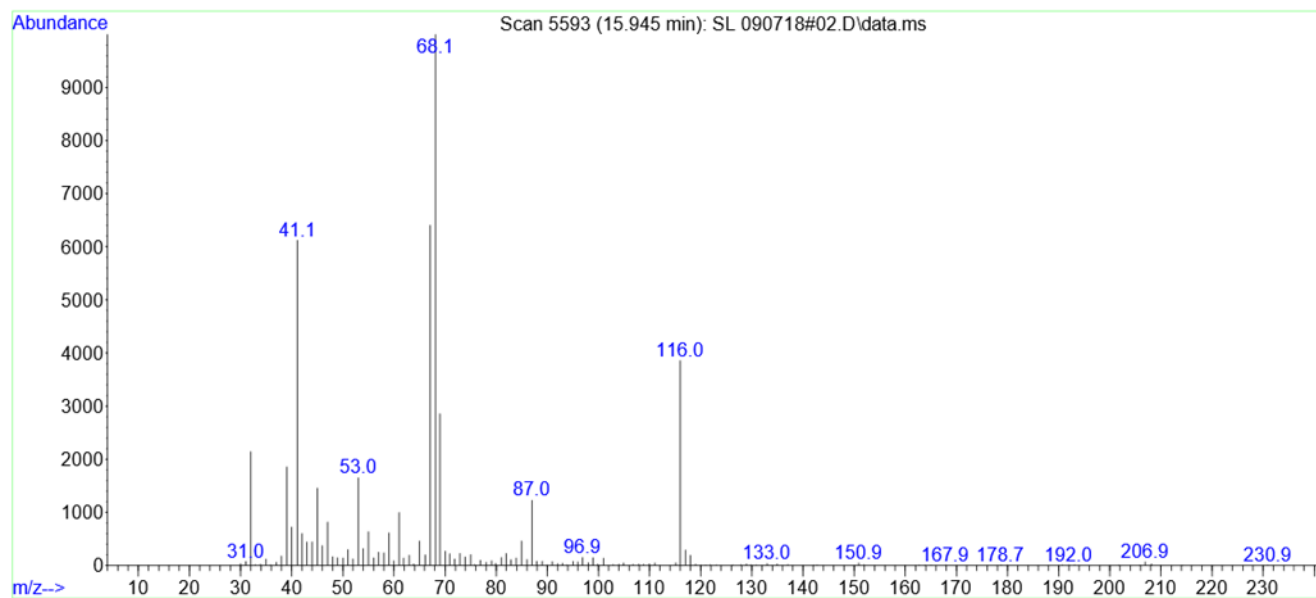
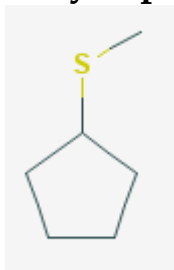
## 7. Cyclopropane isothiocyanate



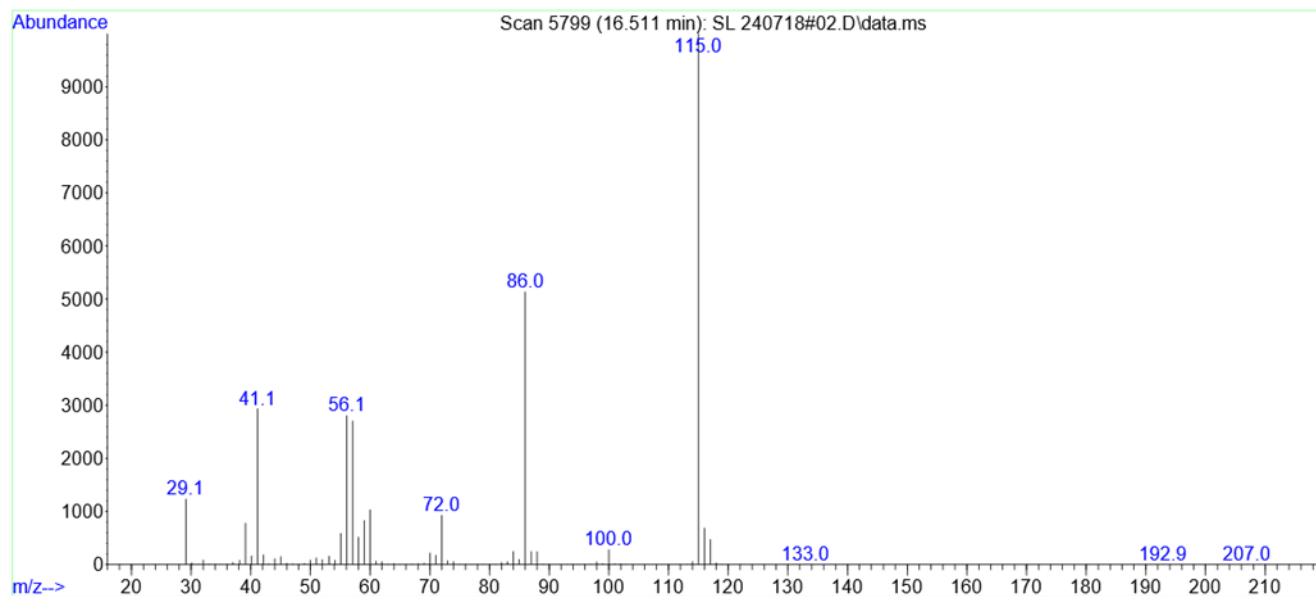
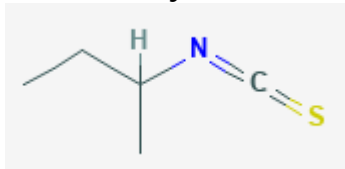
Library Searched : C:\Database\NIST11.L  
Quality : 80  
ID : Cyclopropane, isothiocyanato-



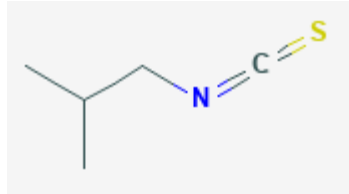
## 8. Cyclopentyl-1-thiaethane



## 9. Sec-butyl isothiocyanate



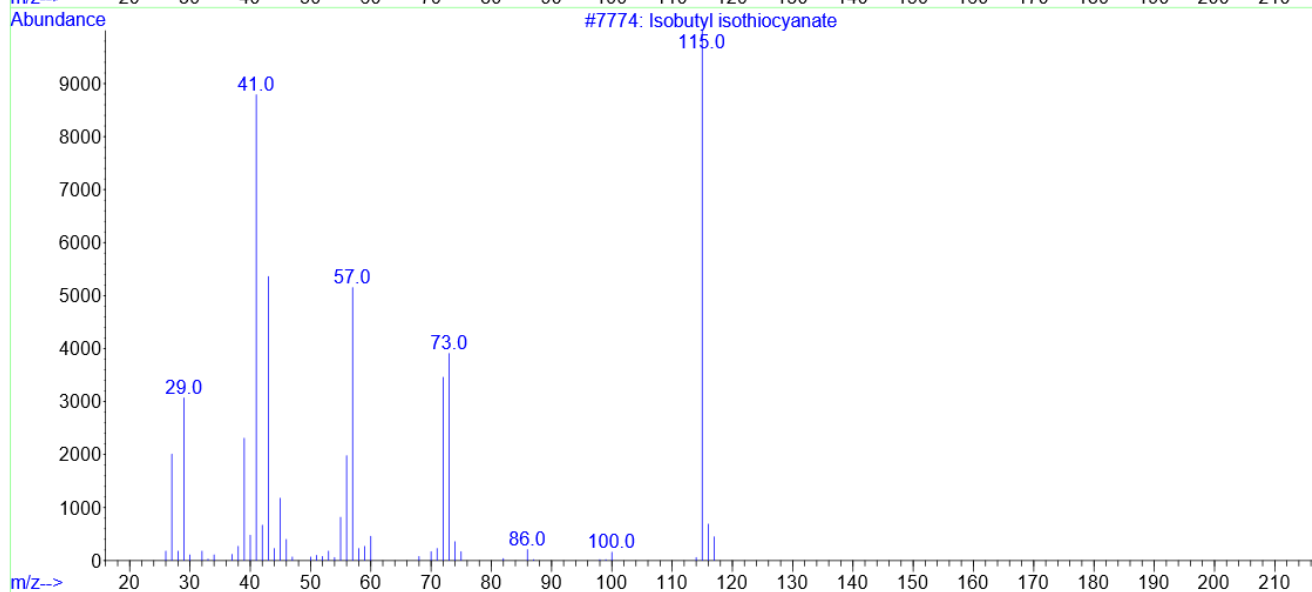
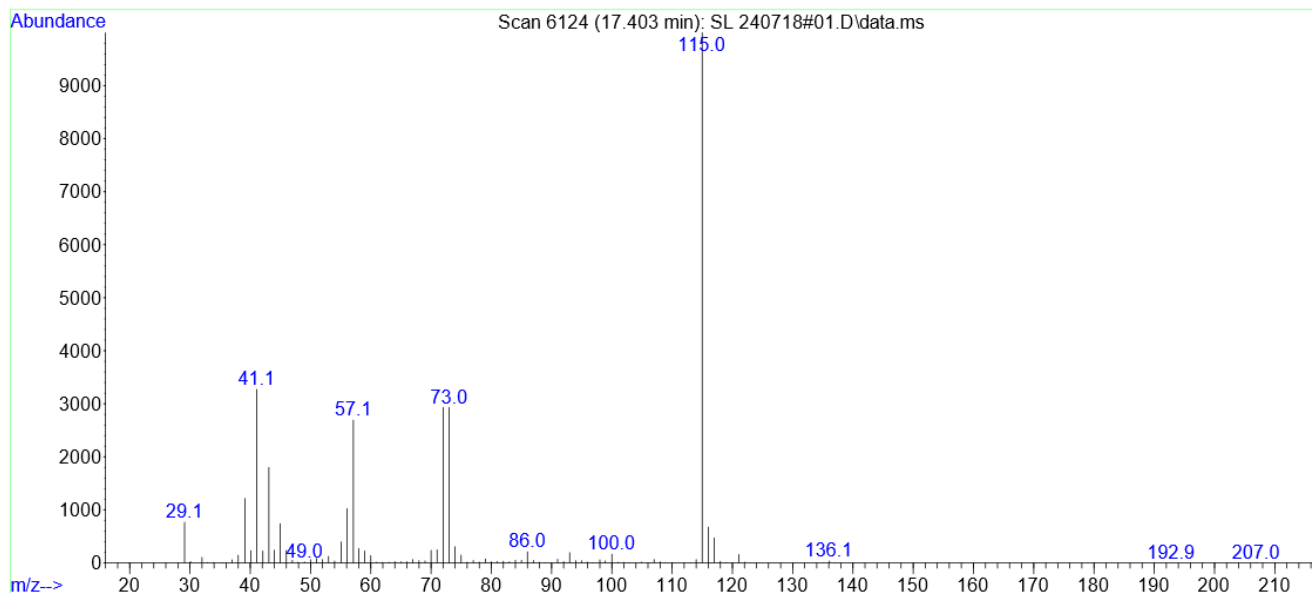
## 10. Isobutyl isothiocyanate



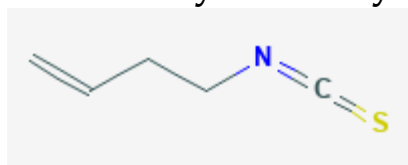
Library Searched : C:\Database\NIST11.L

Quality : 91

ID : Isobutyl isothiocyanate



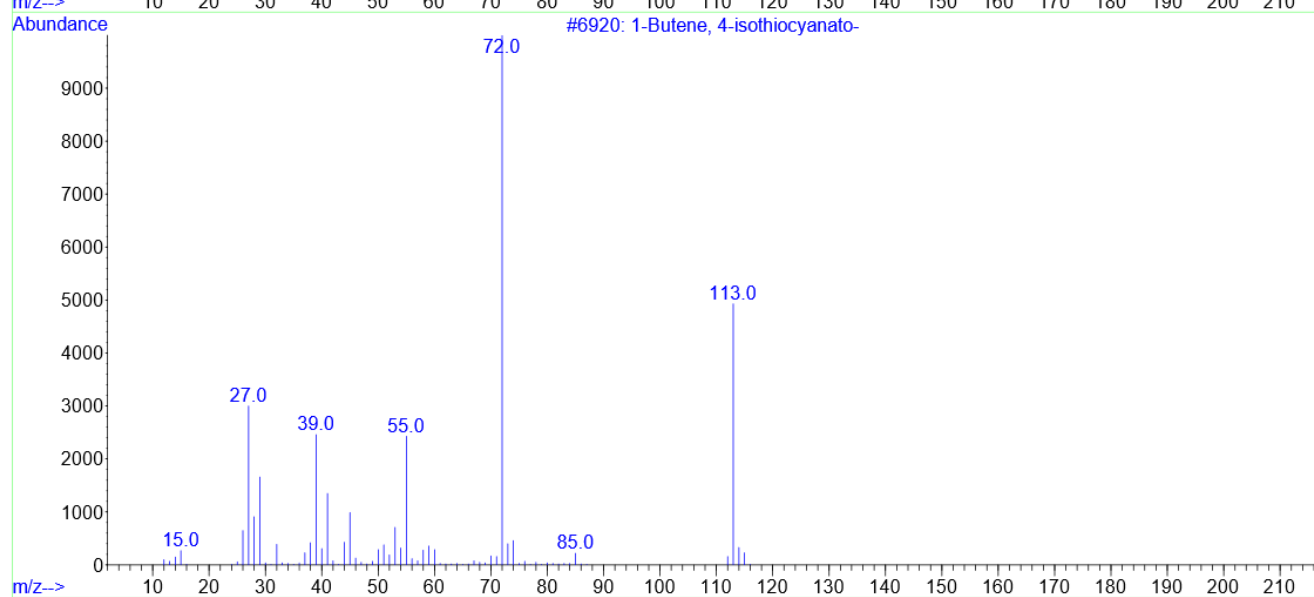
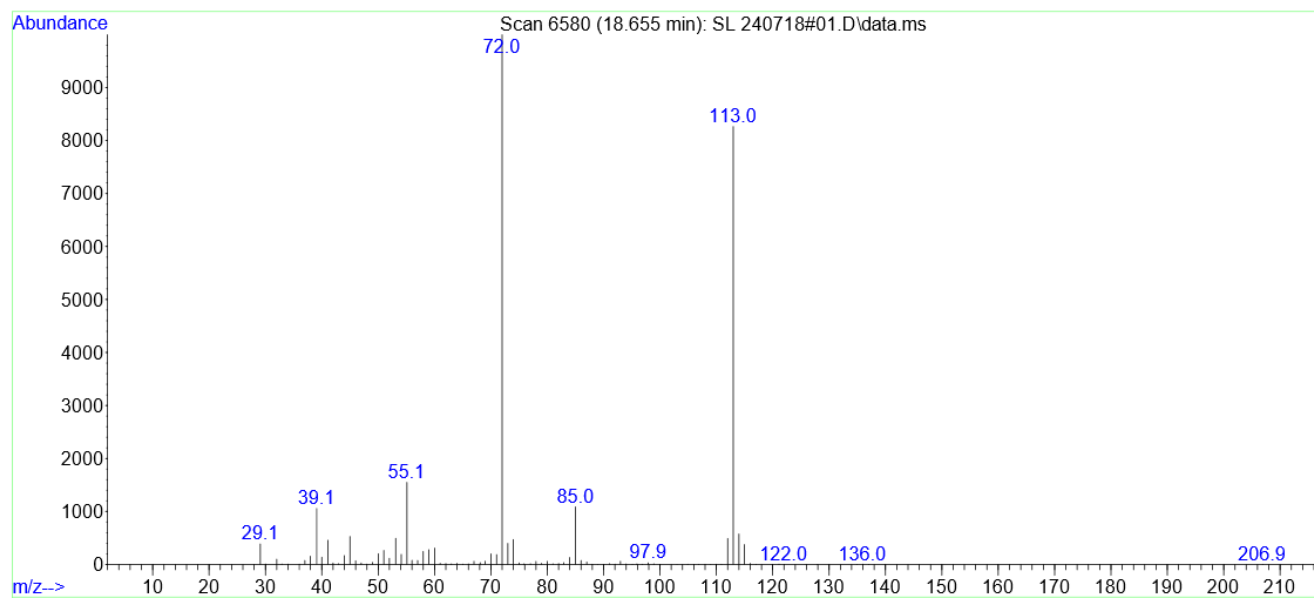
## 11. 3-butenyl isothiocyanate



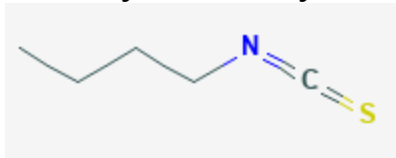
Library Searched : C:\Database\NIST11.L

Quality : 87

ID : 1-Butene, 4-isothiocyanato-



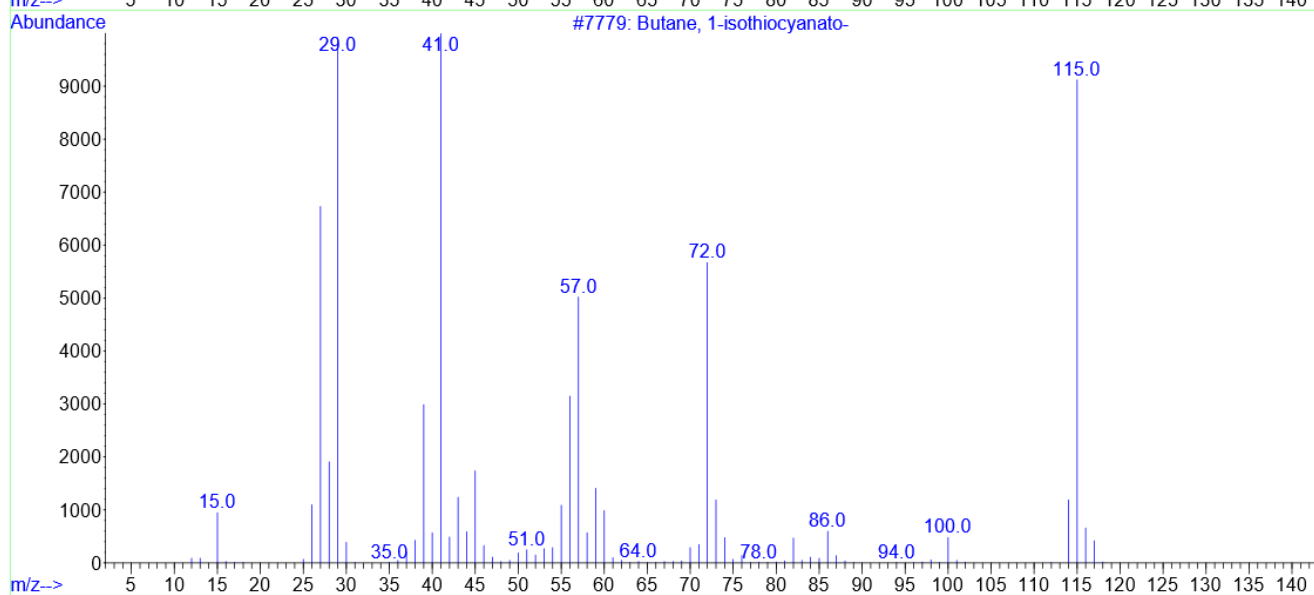
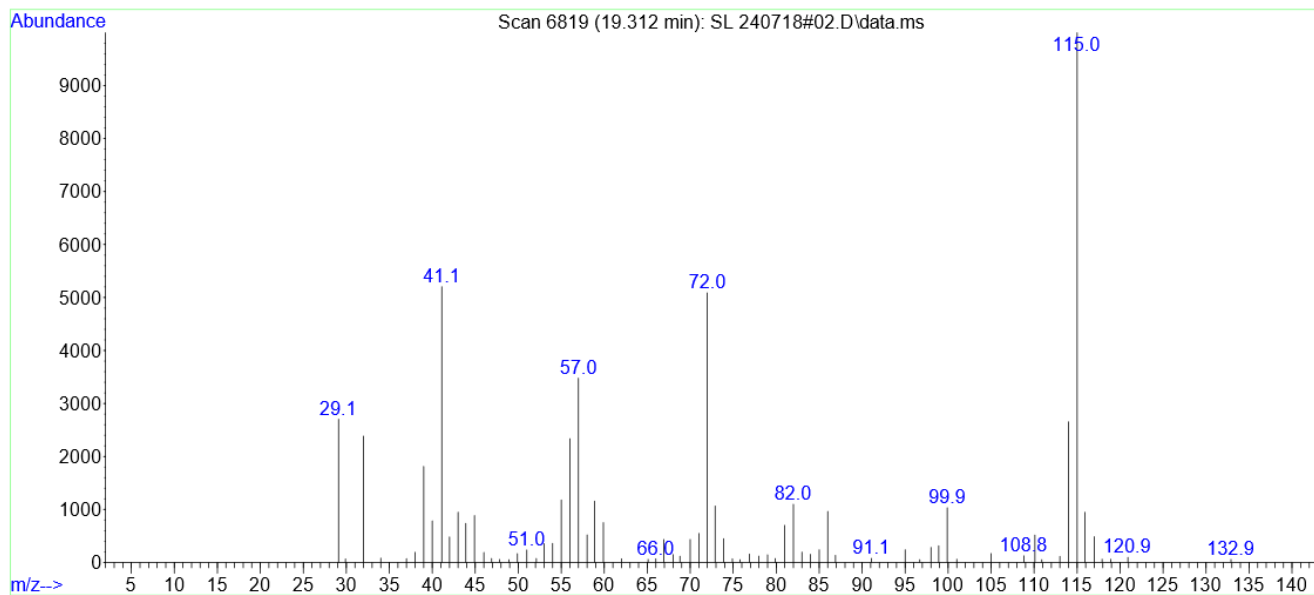
## 12. Butyl isothiocyanate



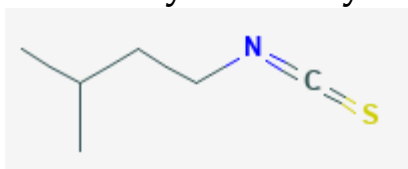
Library Searched : C:\Database\NIST11.L

Quality : 94

ID : Butane, 1-isothiocyanato-



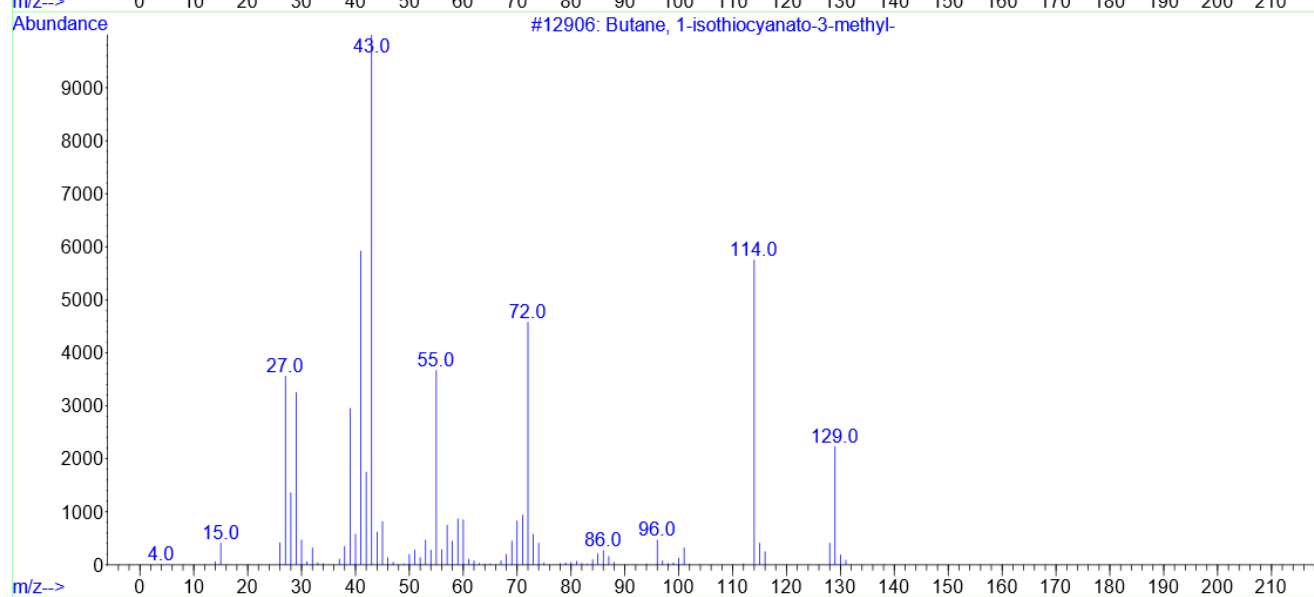
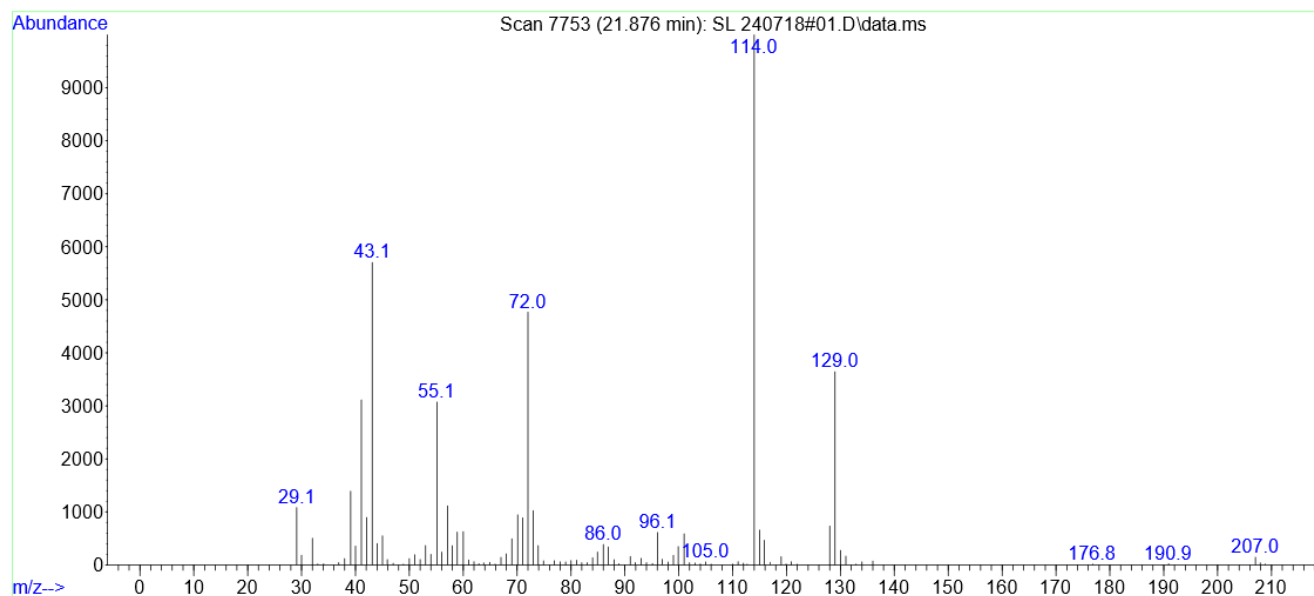
### 13. Isoamyl isothiocyanate



Library Searched : C:\Database\NIST11.L

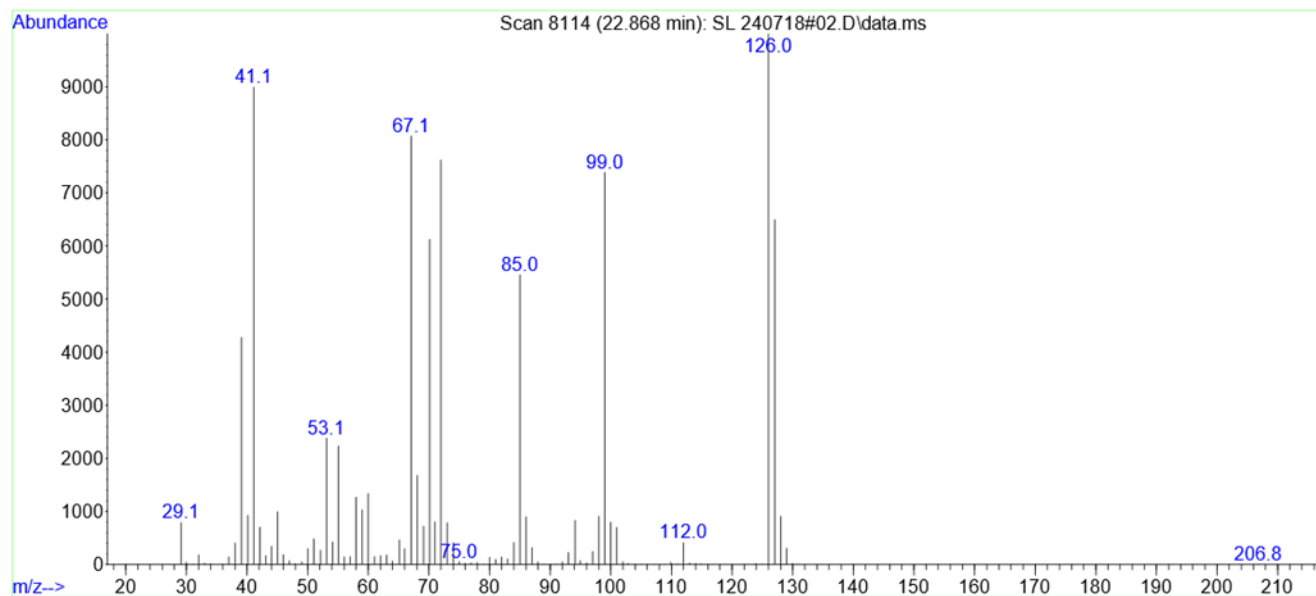
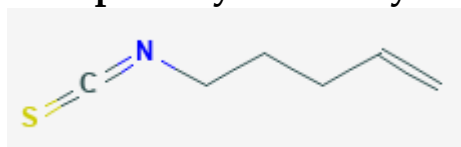
Quality : 87

ID : Butane, 1-isothiocyanato-3-methyl-

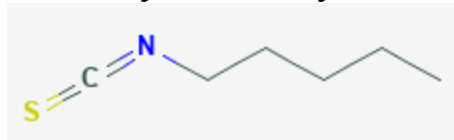




## 14. 4-pentenyl isothiocyanate



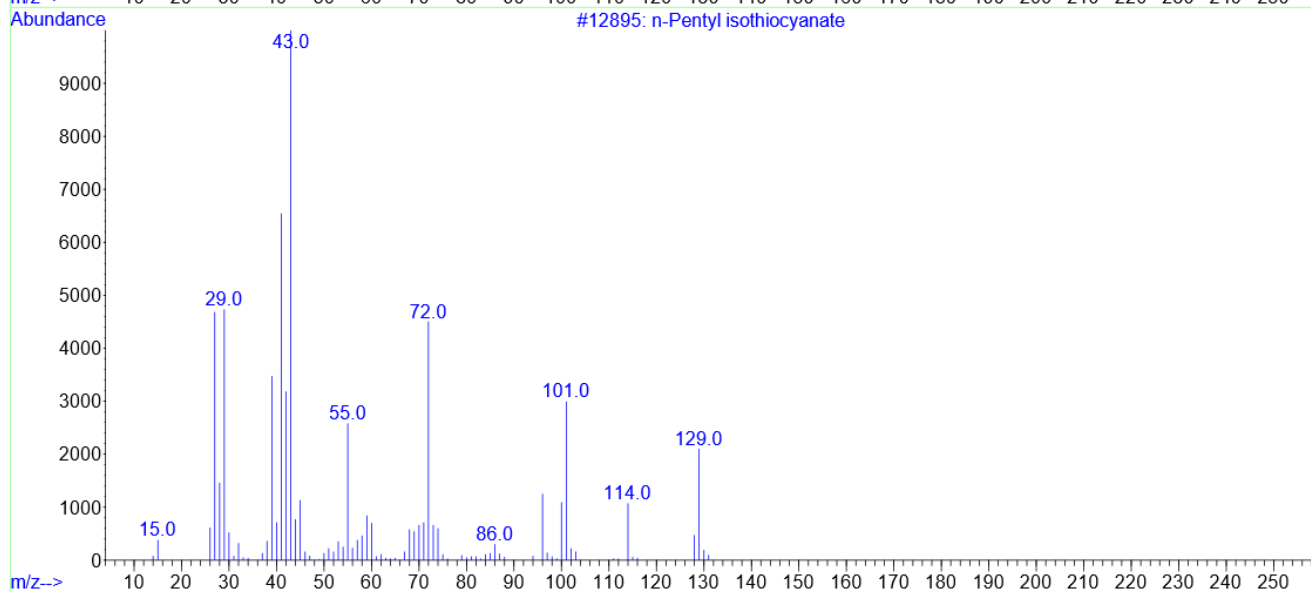
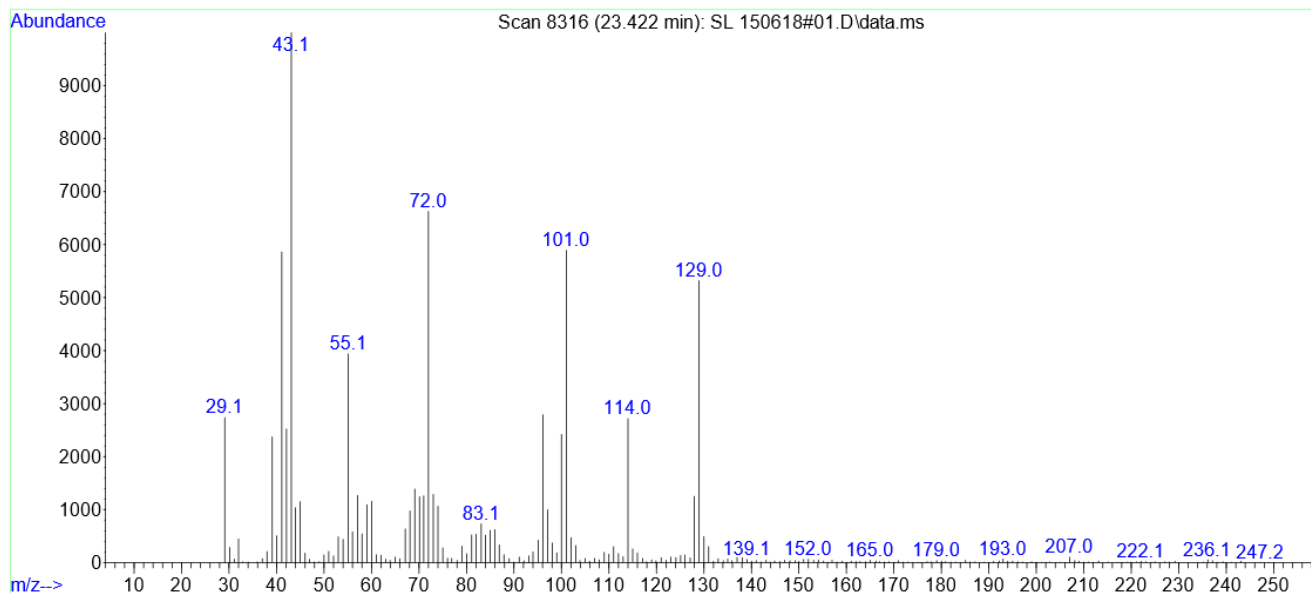
## 15. Pentyl isothiocyanate



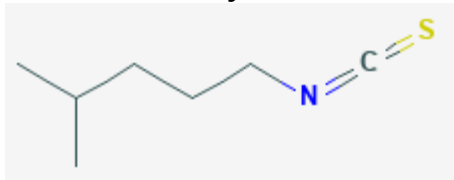
Library Searched : C:\Database\NIST11.L

Quality : 94

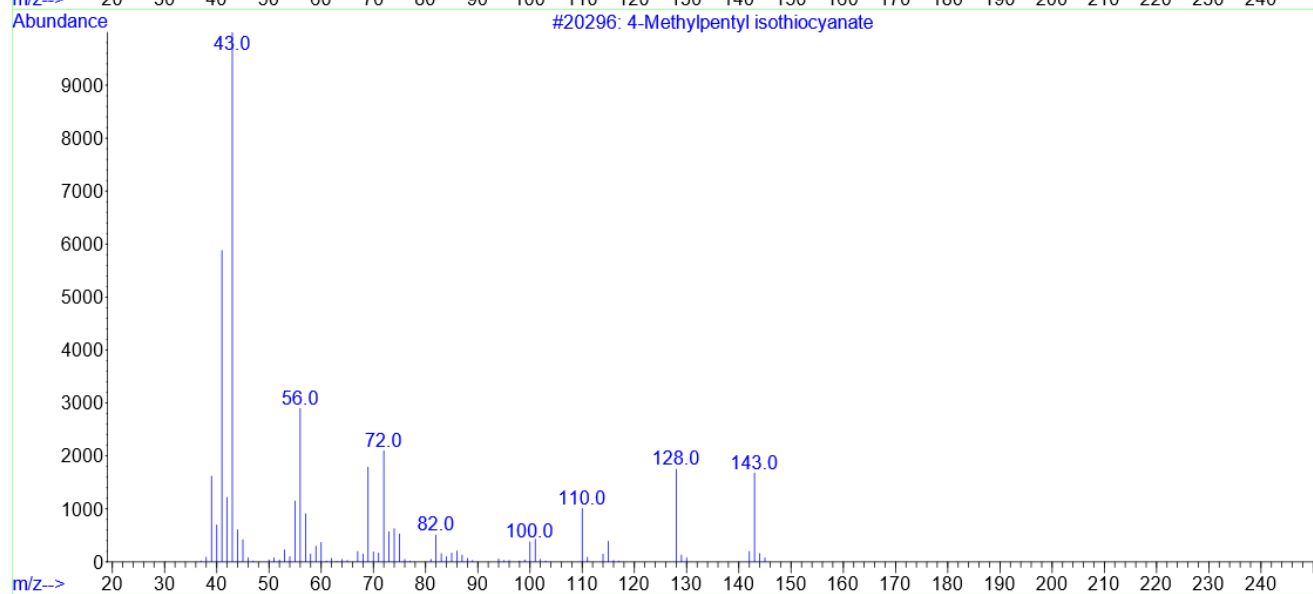
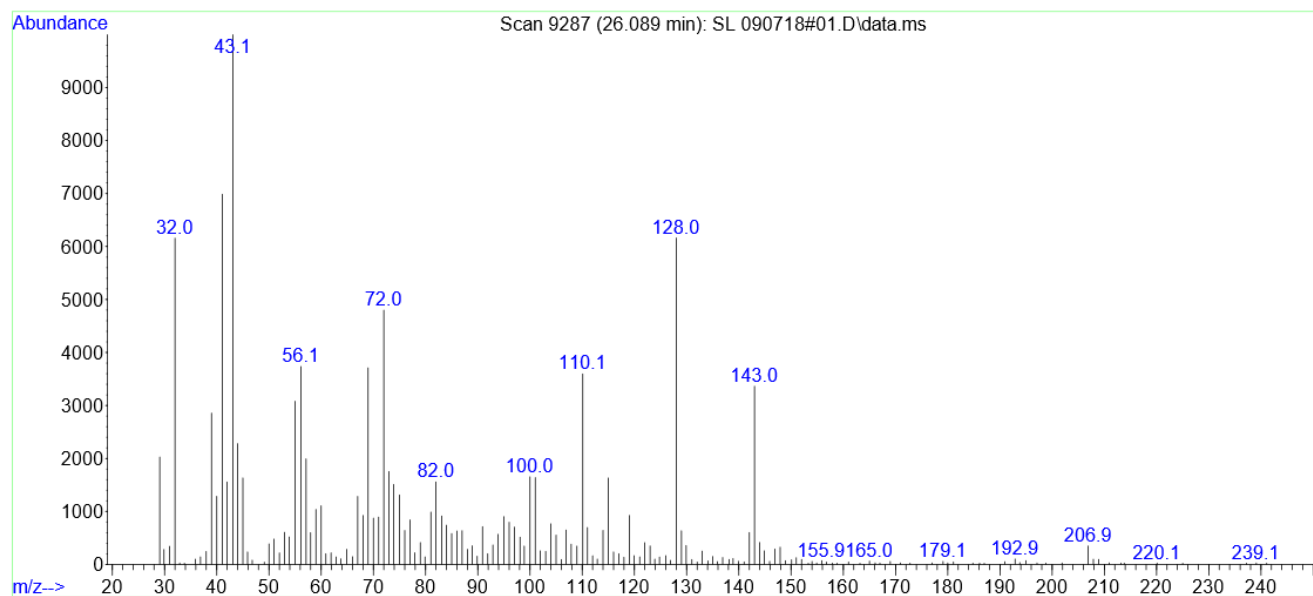
ID : n-Pentyl isothiocyanate



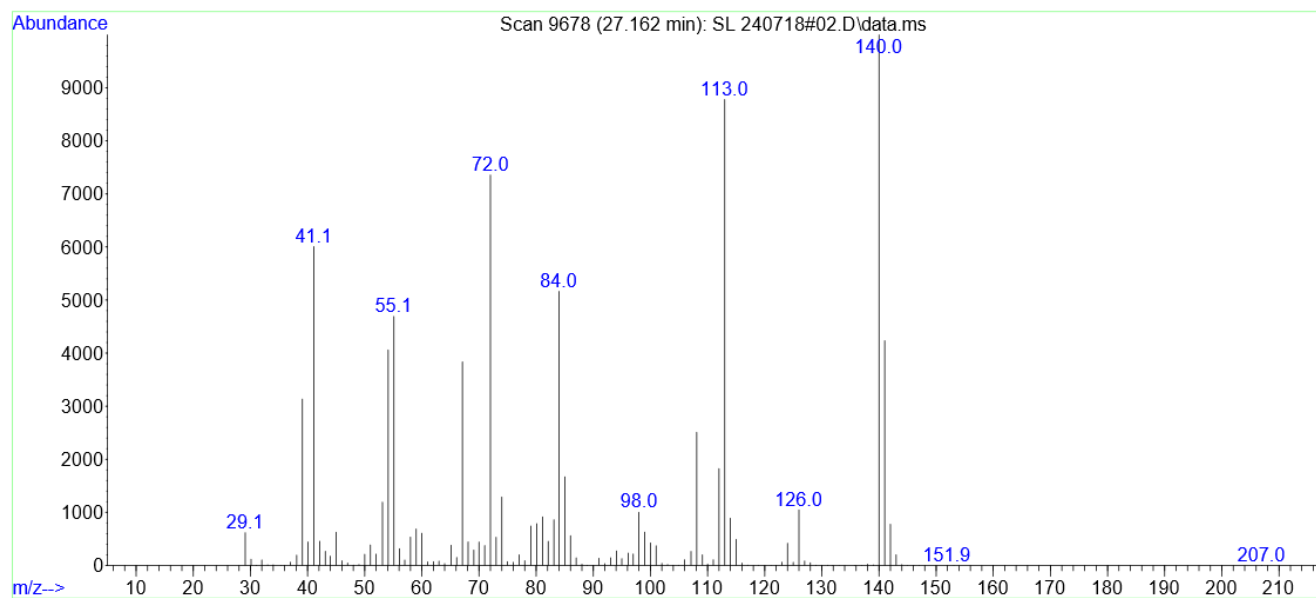
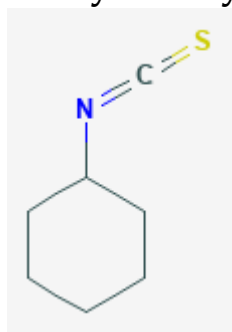
## 16. 1-isothiocyanato-4-methylpentane



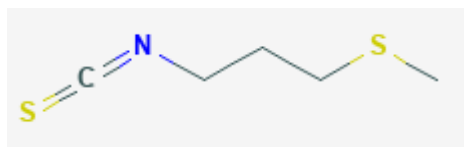
Library Searched : C:\Database\NIST11.L  
Quality : 91  
ID : 4-Methylpentyl isothiocyanate



## 17. Cyclohexyl isothiocyanate



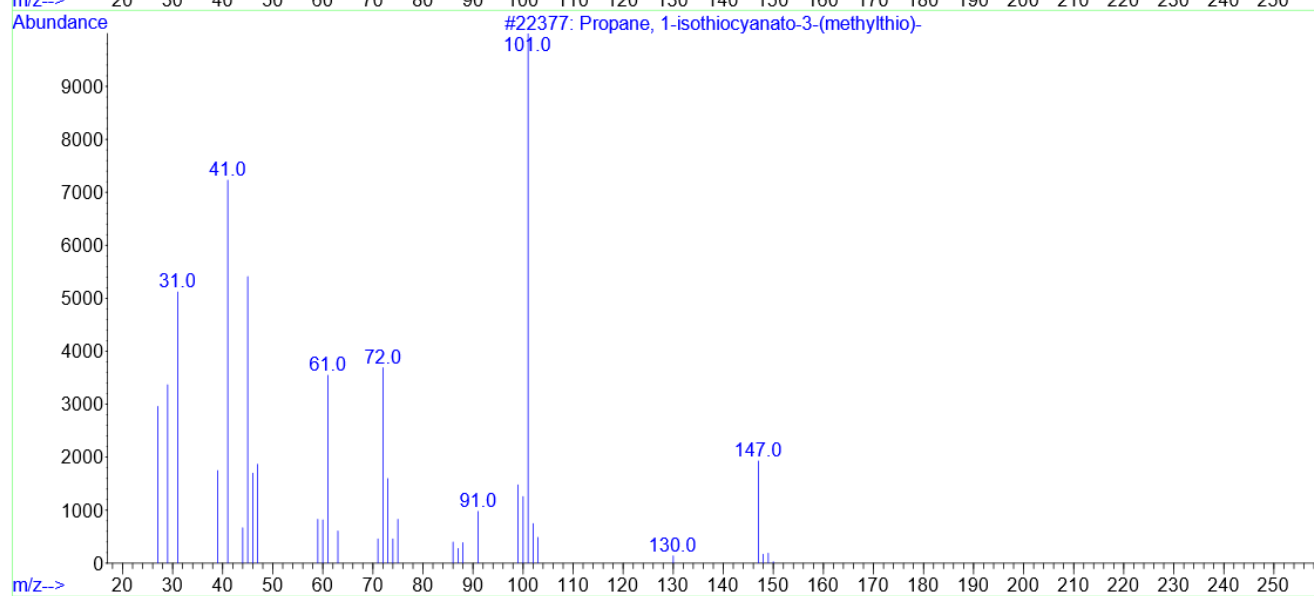
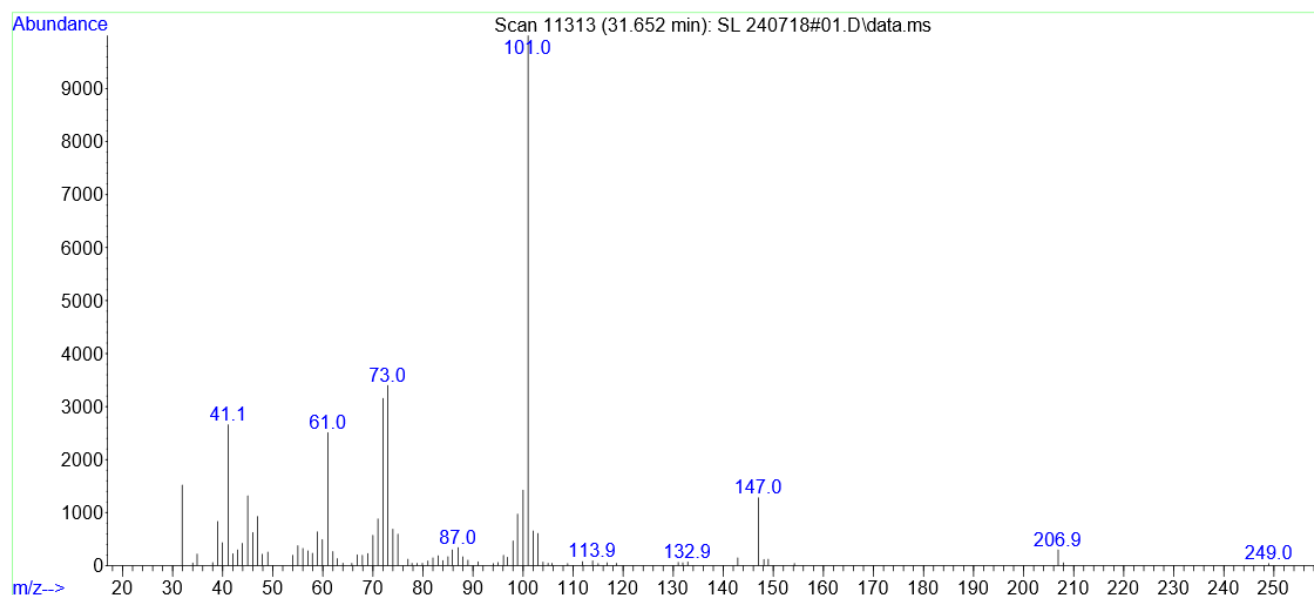
## 19. Iberverin



Library Searched : C:\Database\NIST11.L

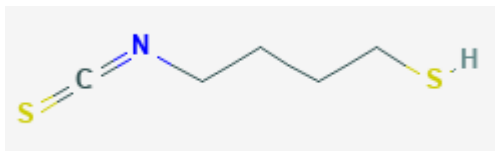
Quality : 83

ID : Propane, 1-isothiocyanato-3-(methylthio)-

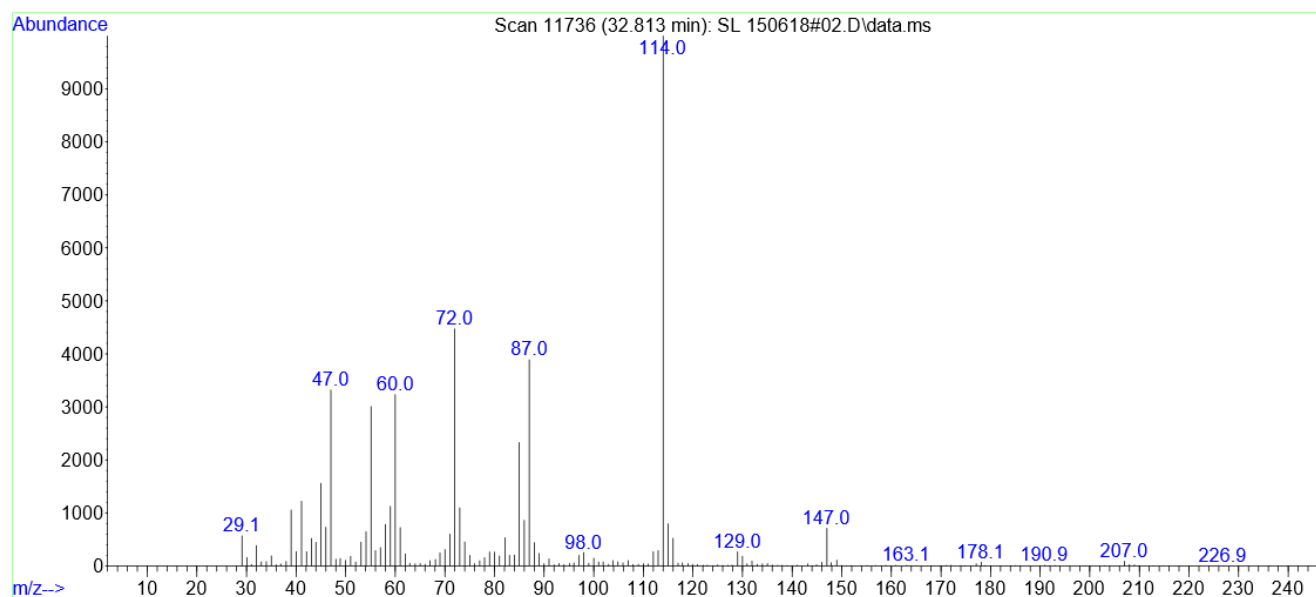
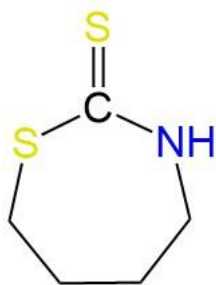


## 20. Sativin

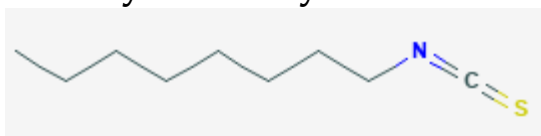
N.B. It is unknown if this is the ITC or tautomer rearrangement of this compound.



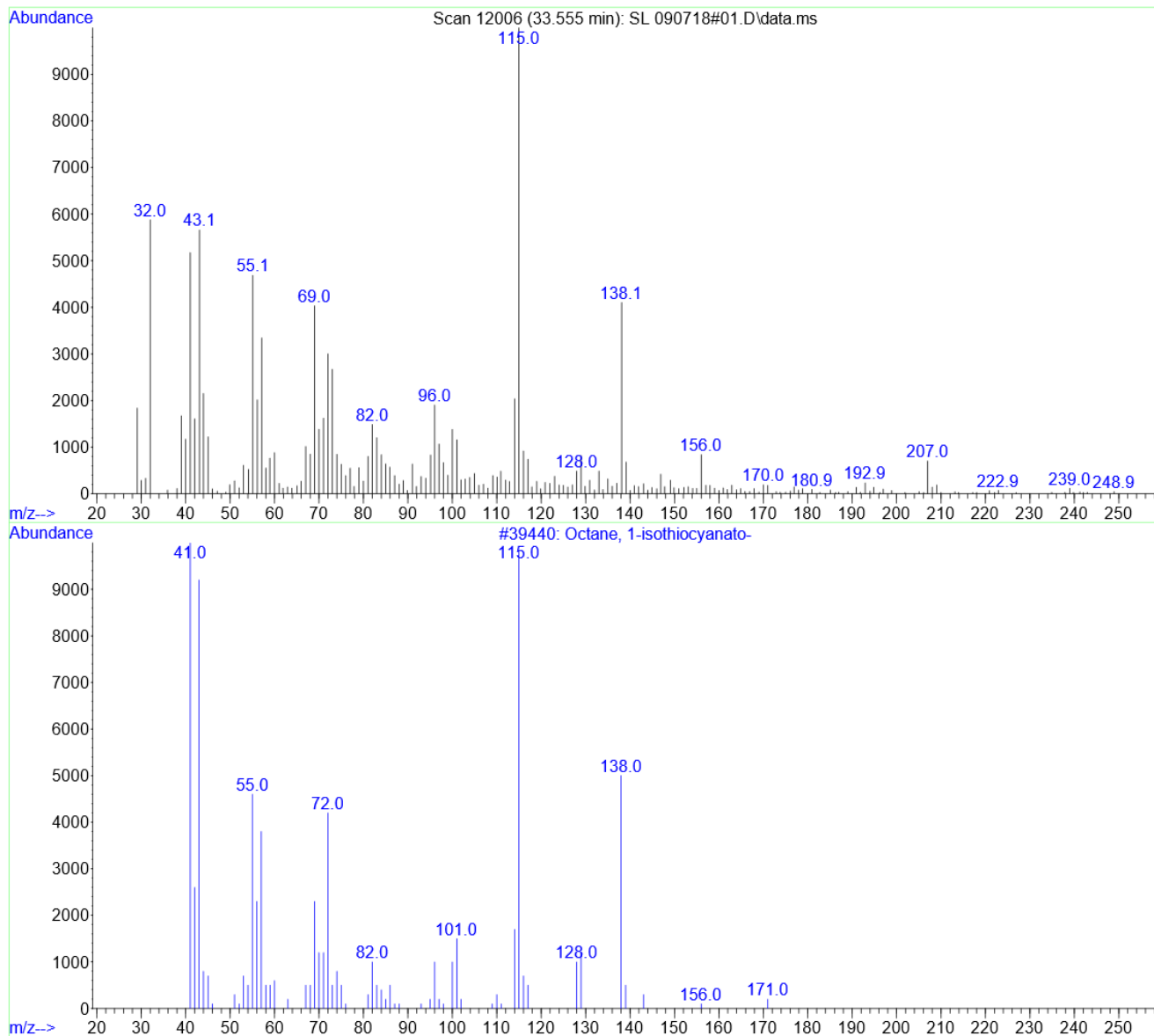
or



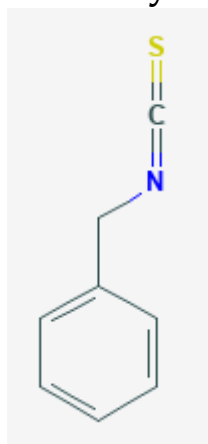
## 21. Octyl isothiocyanate



Library Searched : C:\Database\NIST11.L  
Quality : 53  
ID : Octane, 1-isothiocyanato-



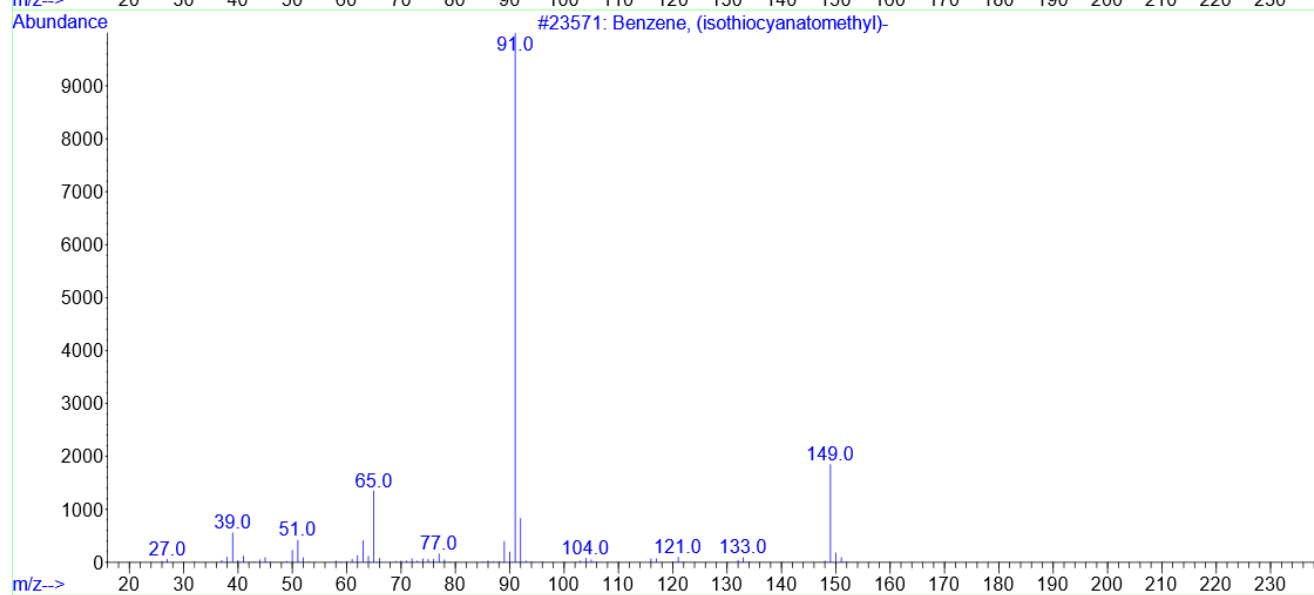
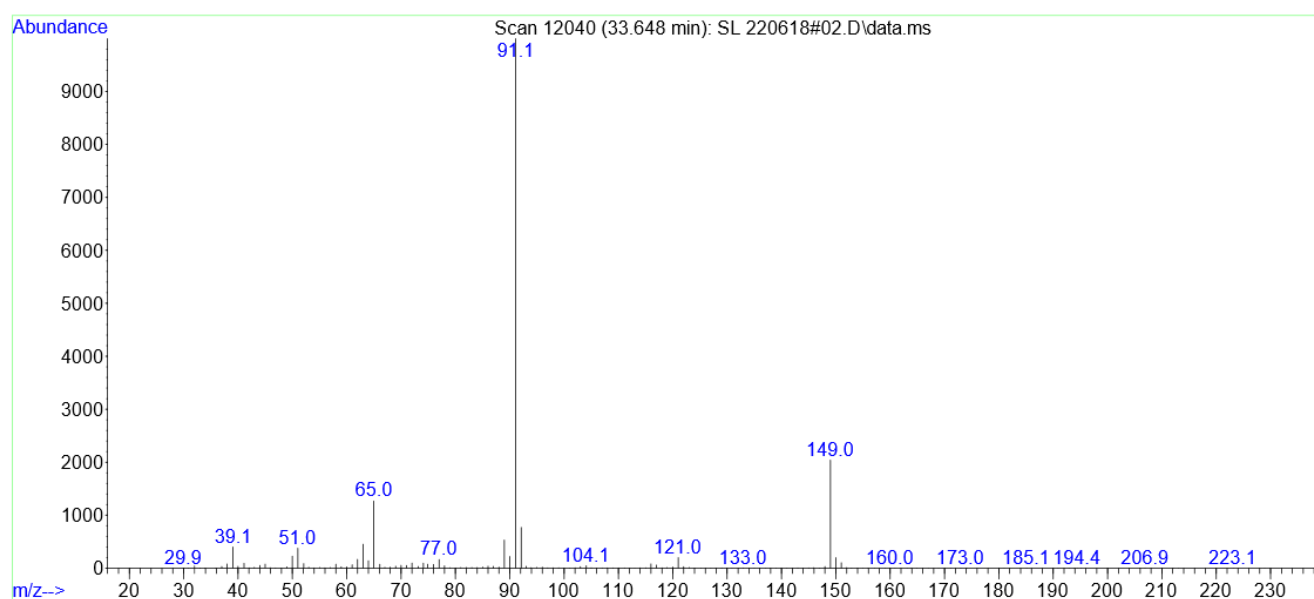
## 22. Benzyl isothiocyanate



Library Searched : C:\Database\NIST11.L

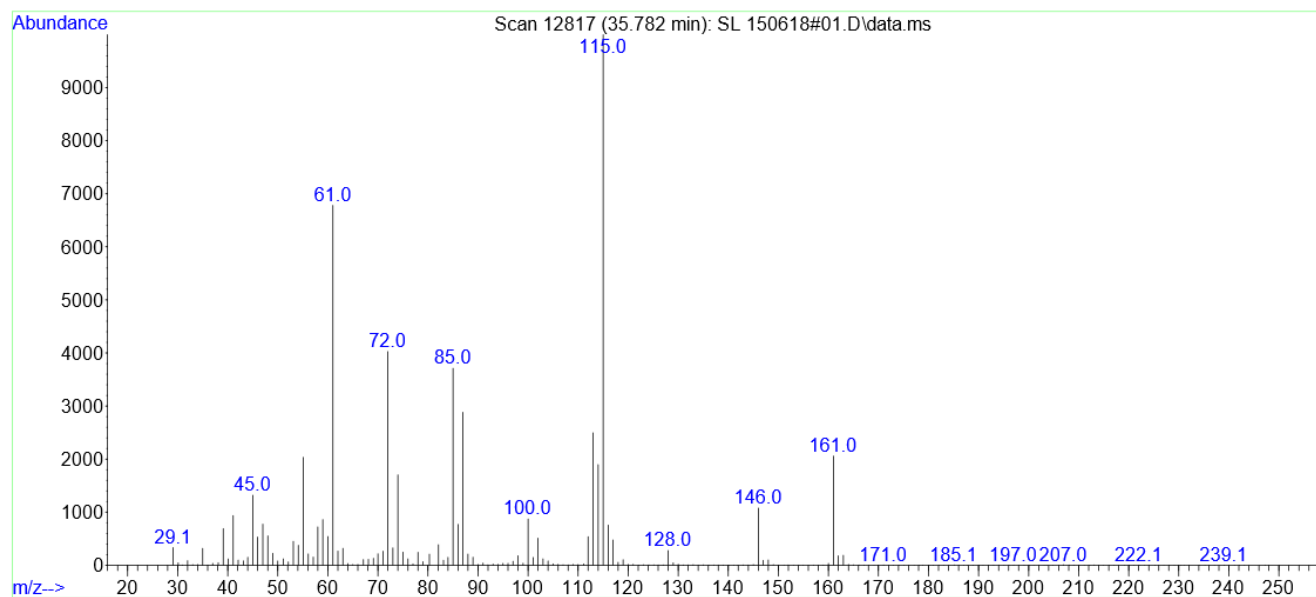
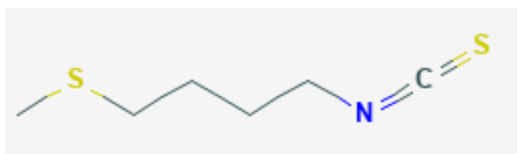
Quality : 91

ID : Benzene, (isothiocyanatomethyl)-

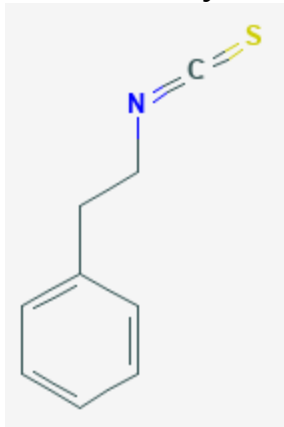




## 23. Erucin



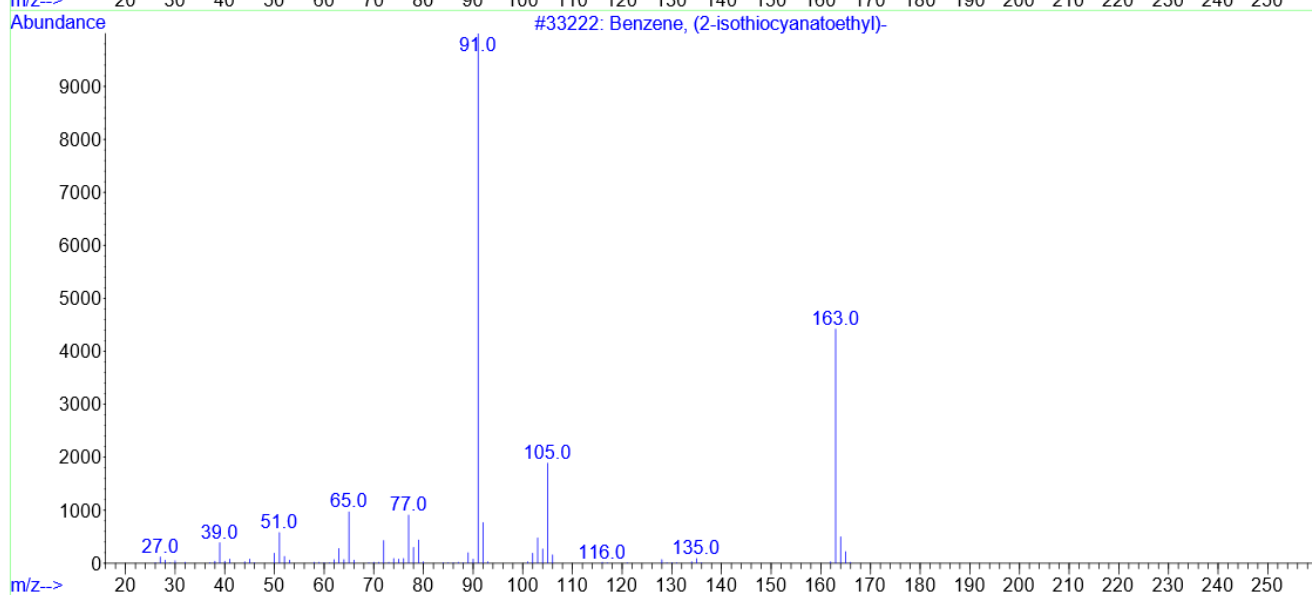
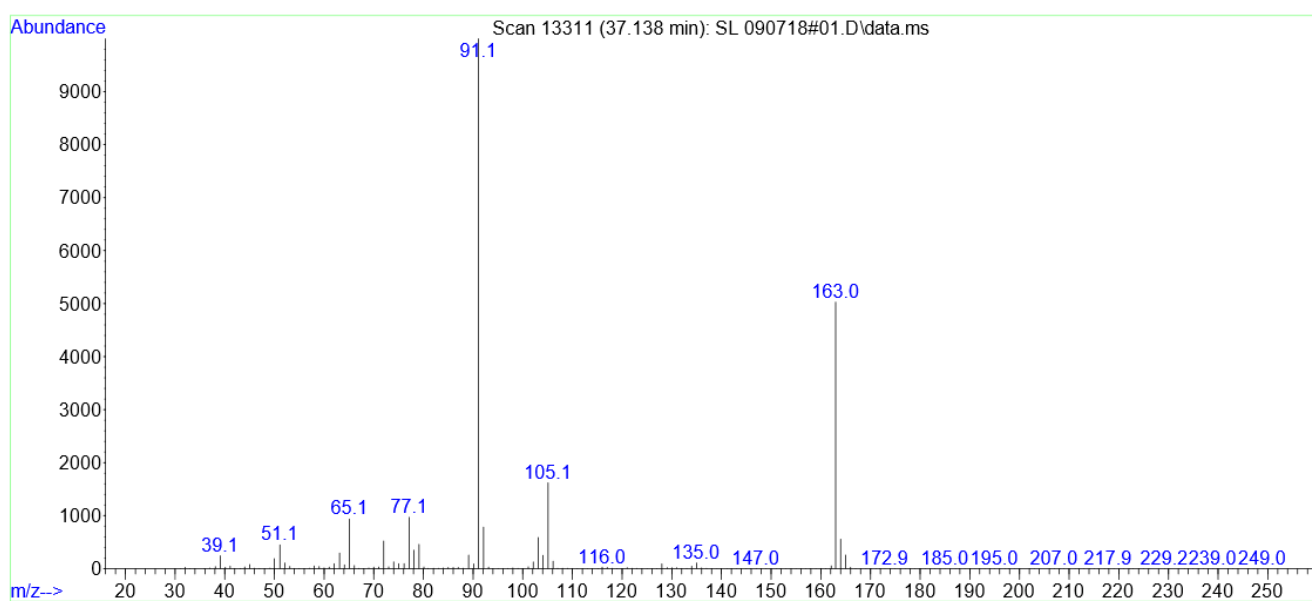
## 24. Phenethyl isothiocyanate



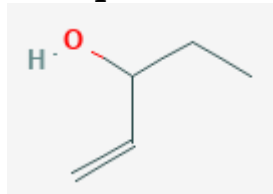
Library Searched : C:\Database\NIST11.L

Quality : 95

ID : Benzene, (2-isothiocyanatoethyl)-



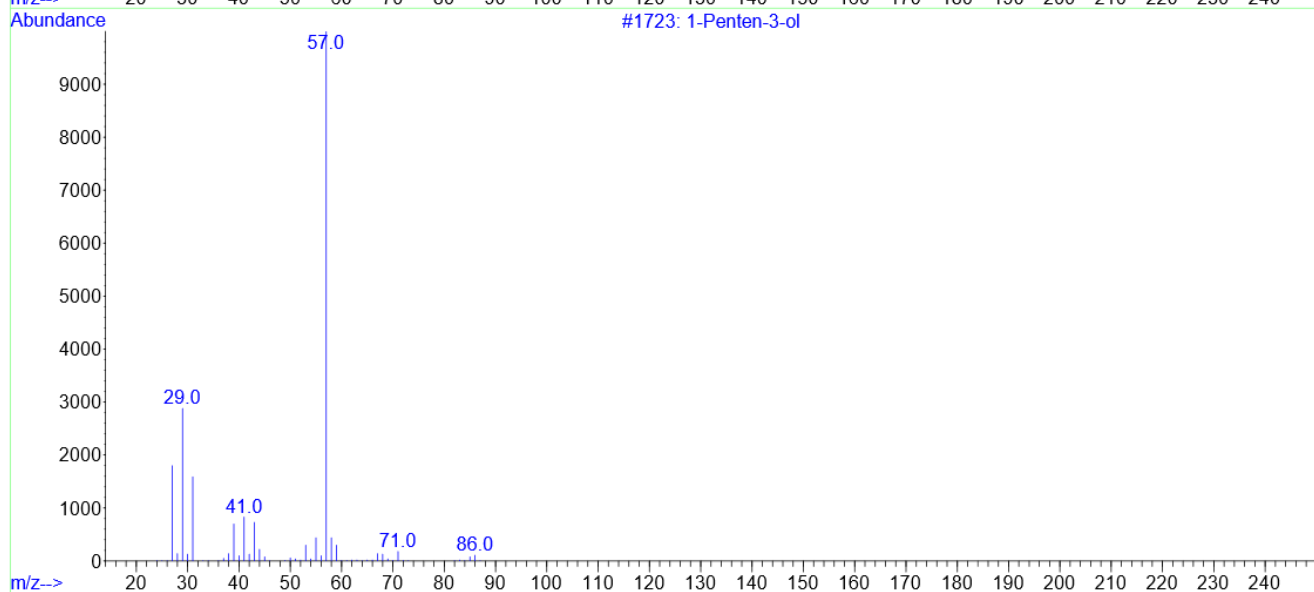
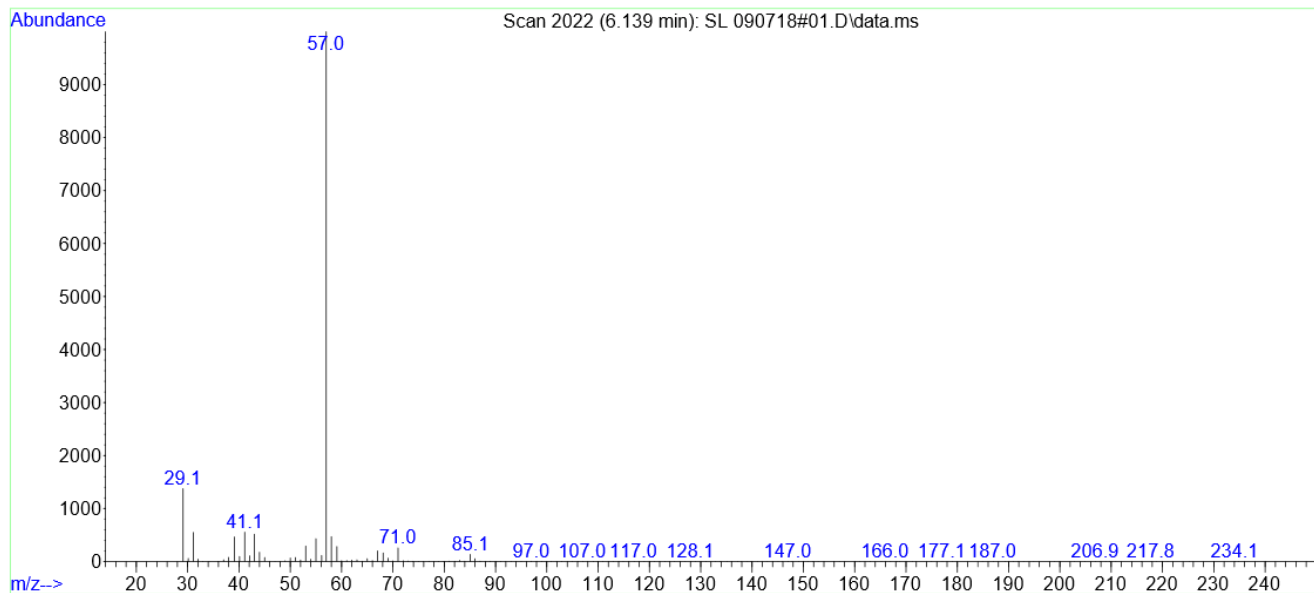
## 25. 1-penten-3-ol



Library Searched : C:\Database\NIST11.L

Quality : 90

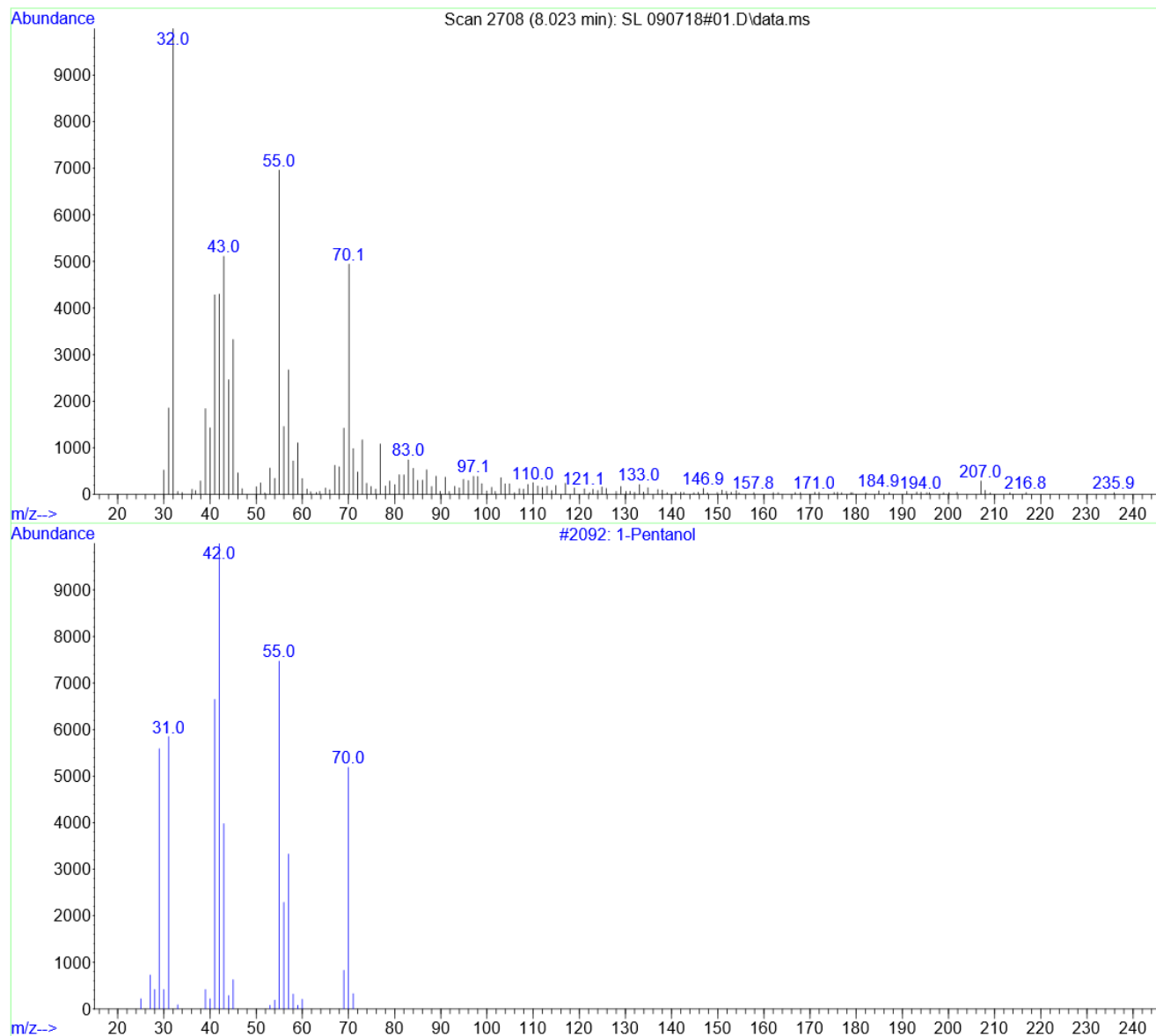
ID : 1-Penten-3-ol



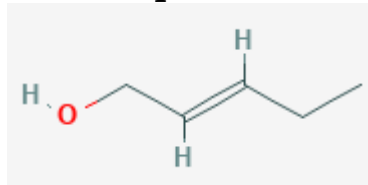
## 26. Pentan-1-ol



Library Searched : C:\Database\NIST11.L  
Quality : 47  
ID : 1-Pentanol



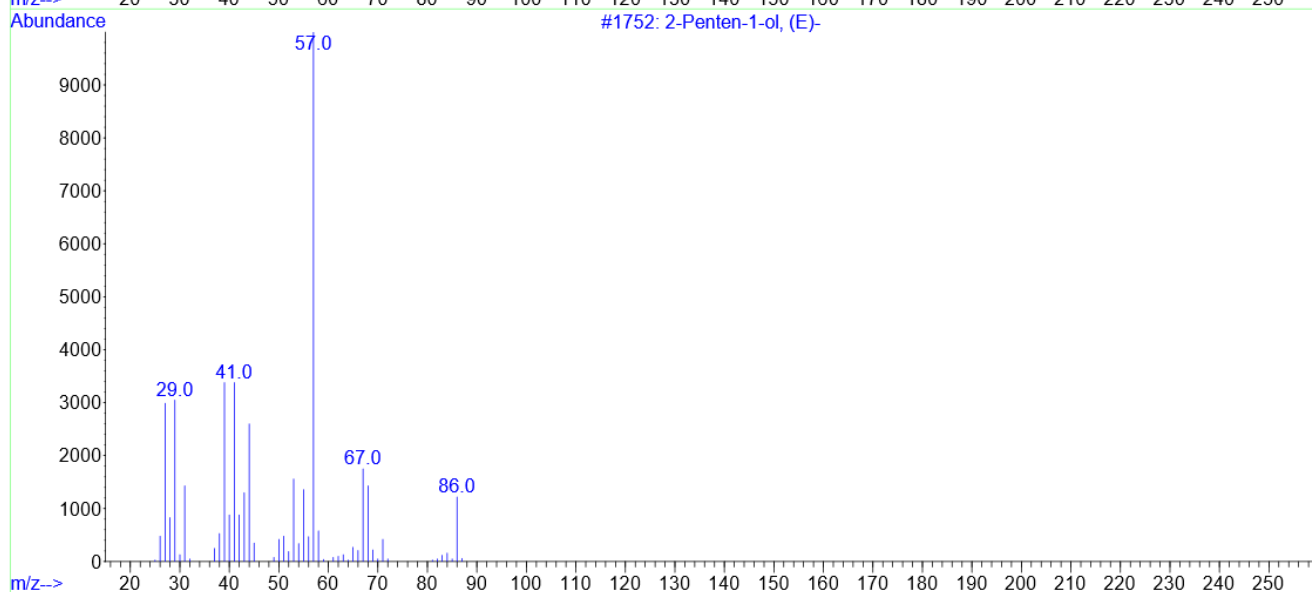
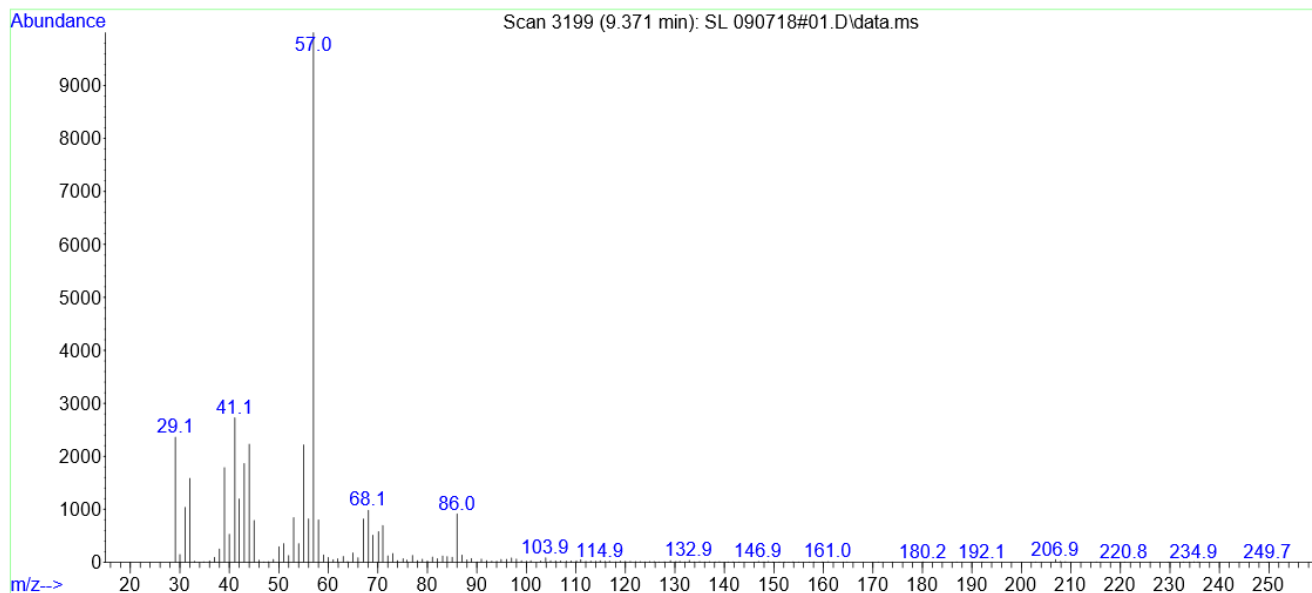
## 27. (E)-2-penten-1-ol



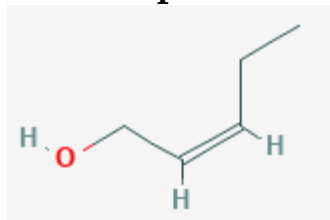
Library Searched : C:\Database\NIST11.L

Quality : 72

ID : 2-Penten-1-ol, (E)-



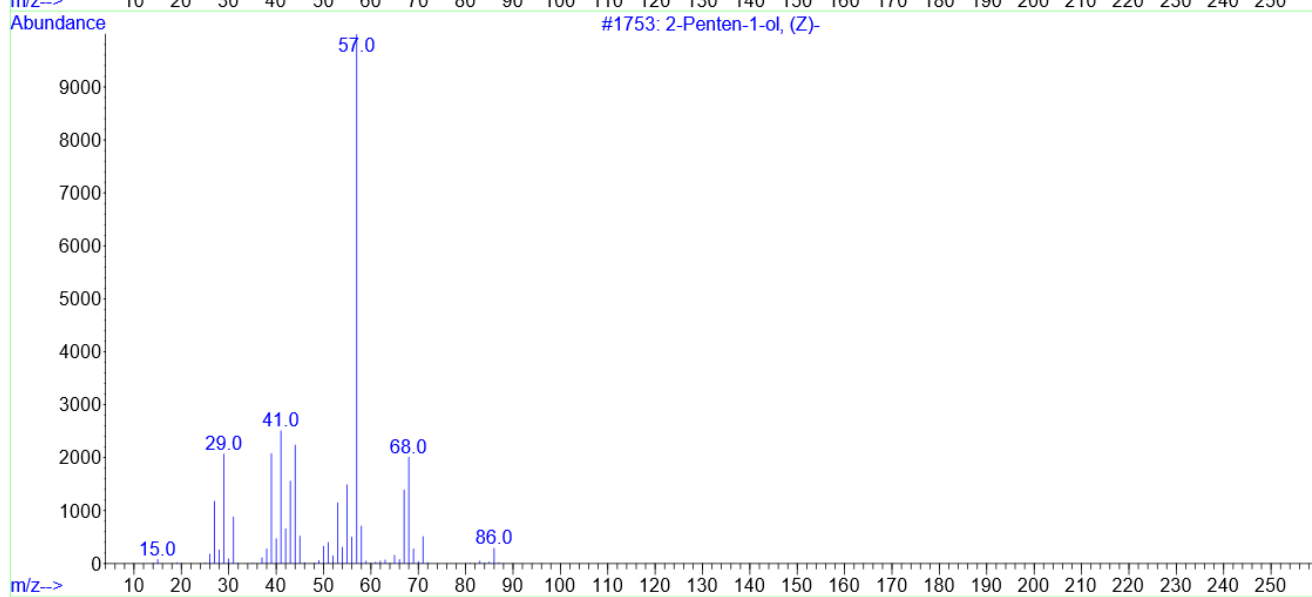
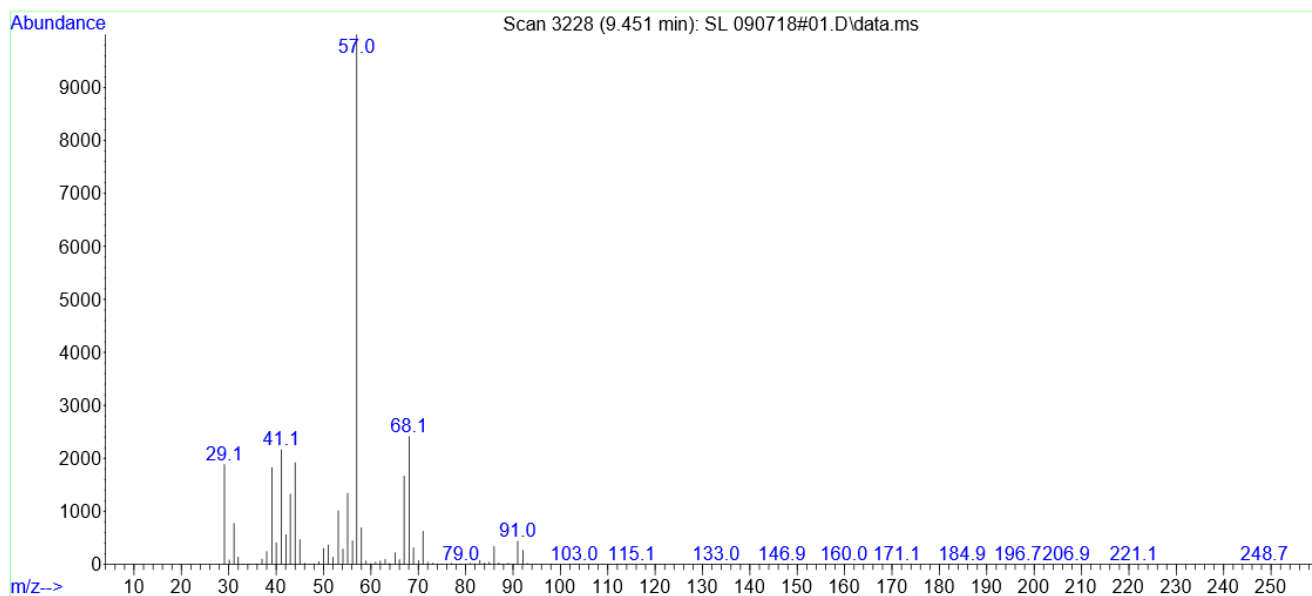
## 28. (Z)-2-penten-1-ol



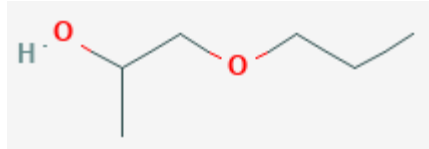
Library Searched : C:\Database\NIST11.L

Quality : 93

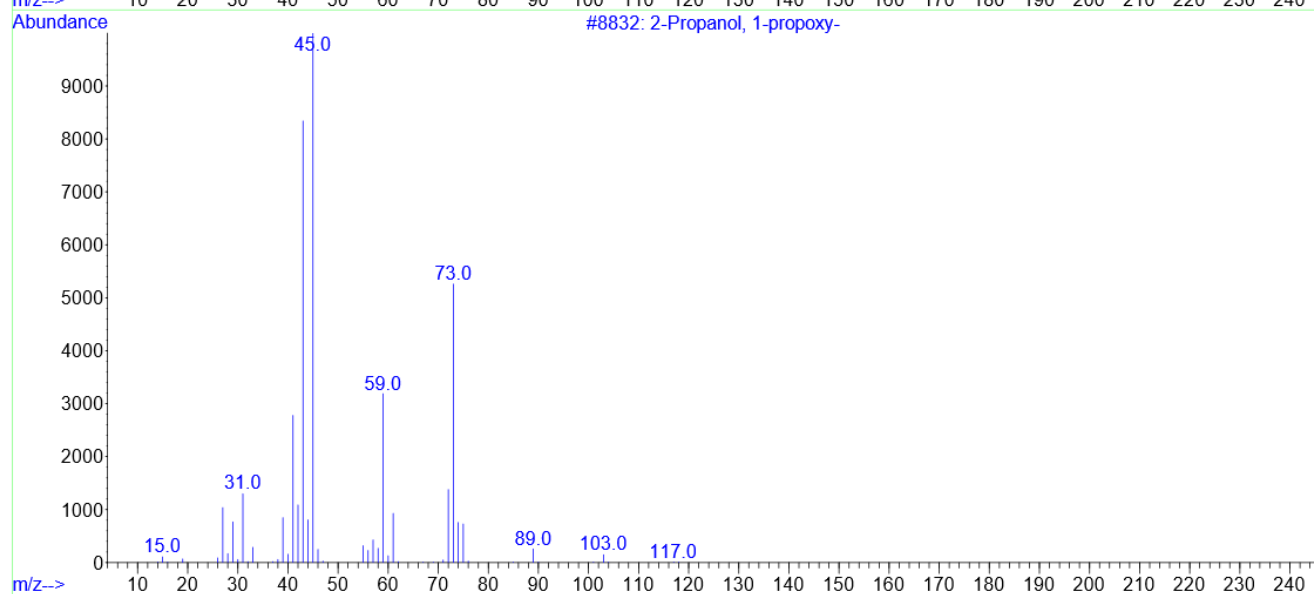
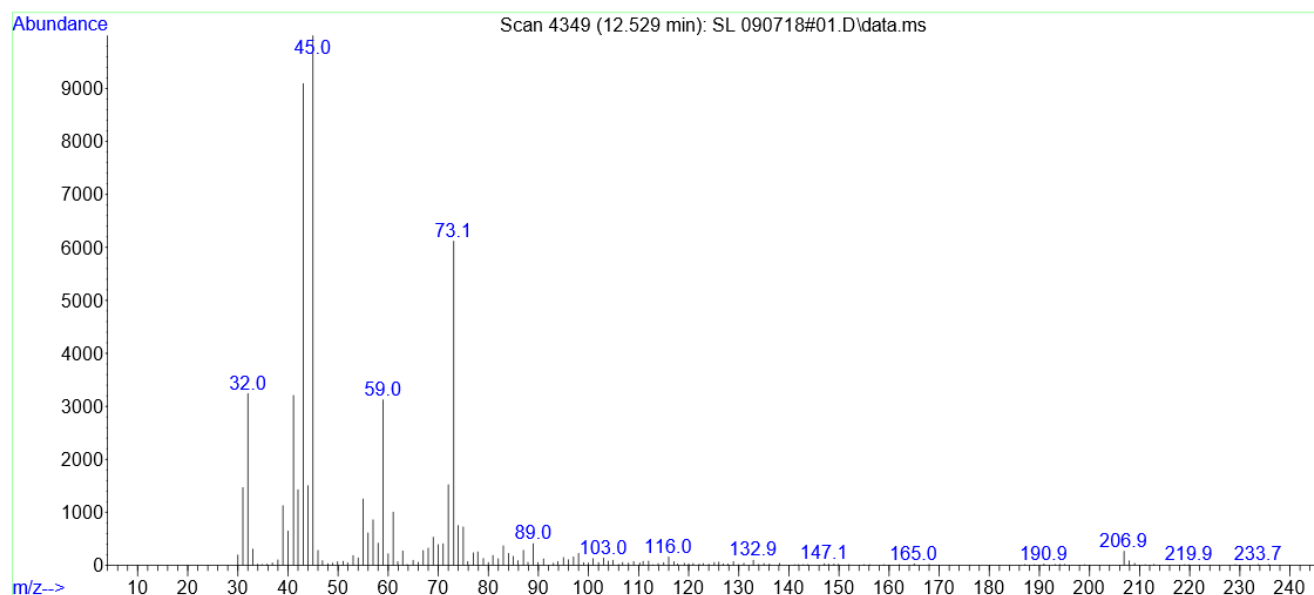
ID : 2-Penten-1-ol, (Z)-



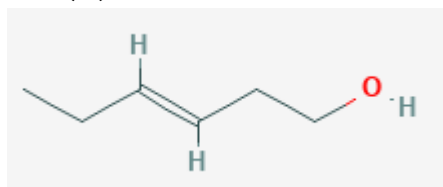
## 29. 1-propoxy-2-propanol



Library Searched : C:\Database\NIST11.L  
Quality : 87  
ID : 2-Propanol, 1-propoxy-



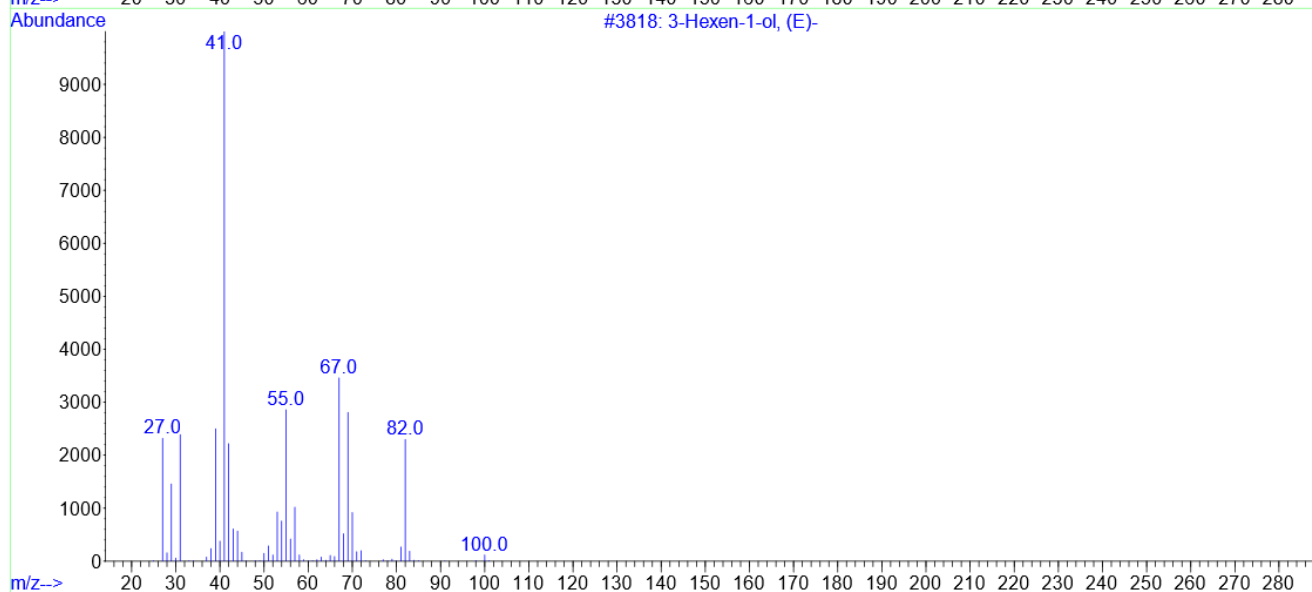
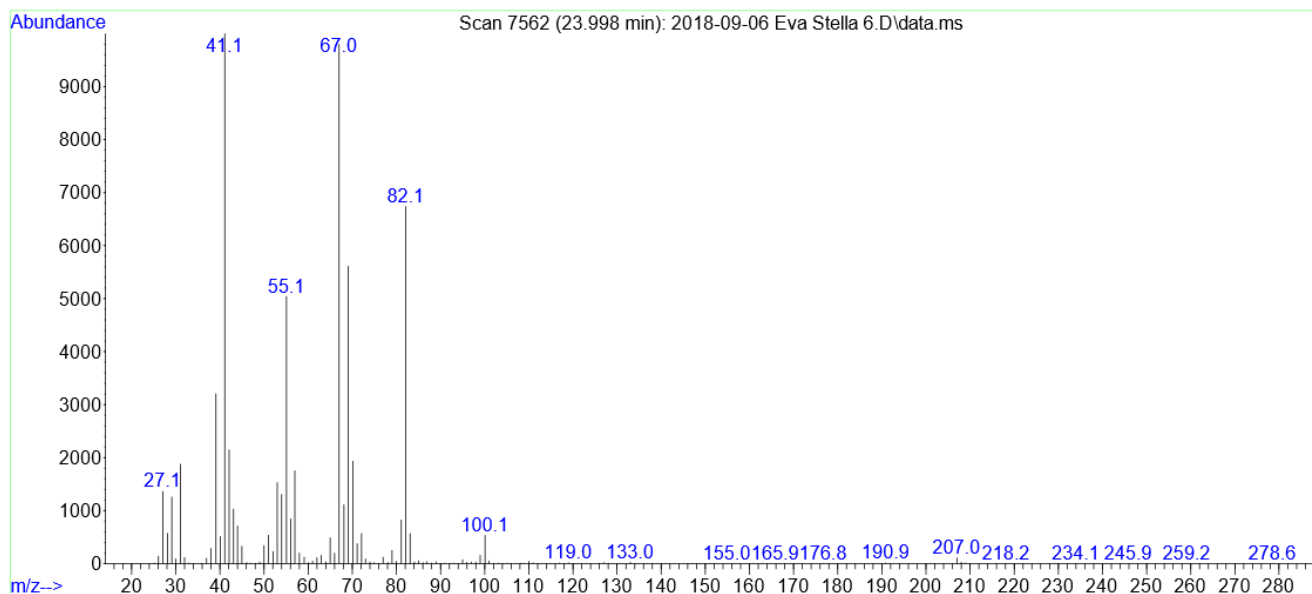
### 30. (E)-3-hexen-1-ol



Library Searched : C:\Database\NIST11.L

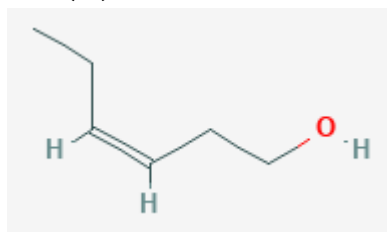
Quality : 95

ID : 3-Hexen-1-ol, (E)-





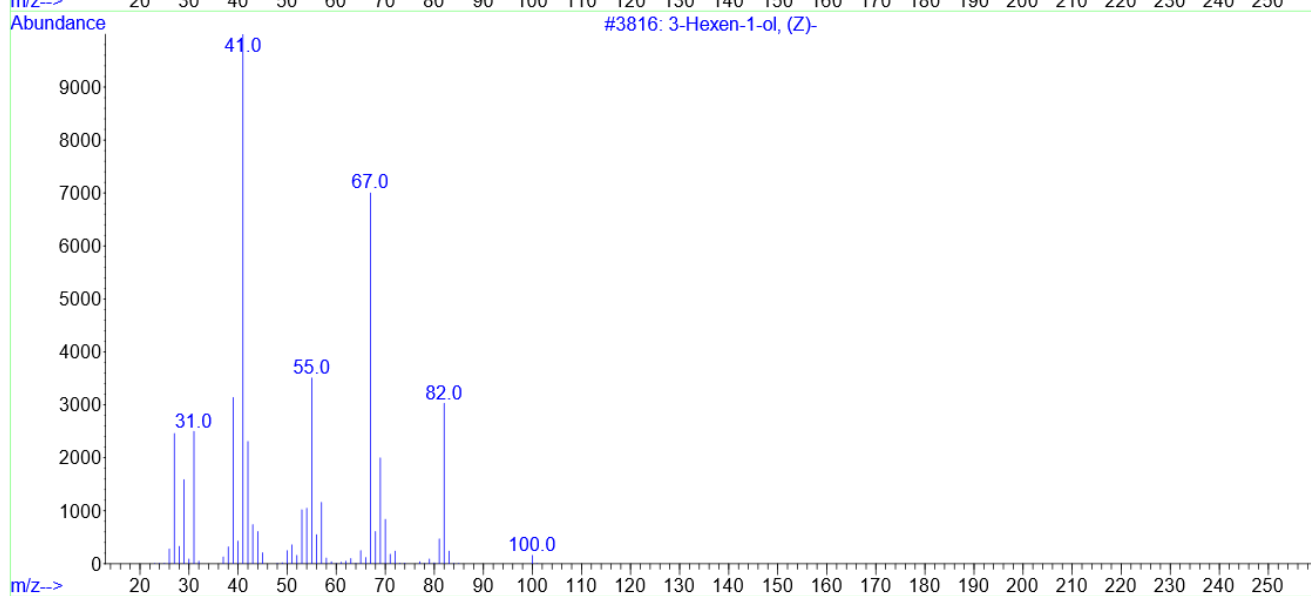
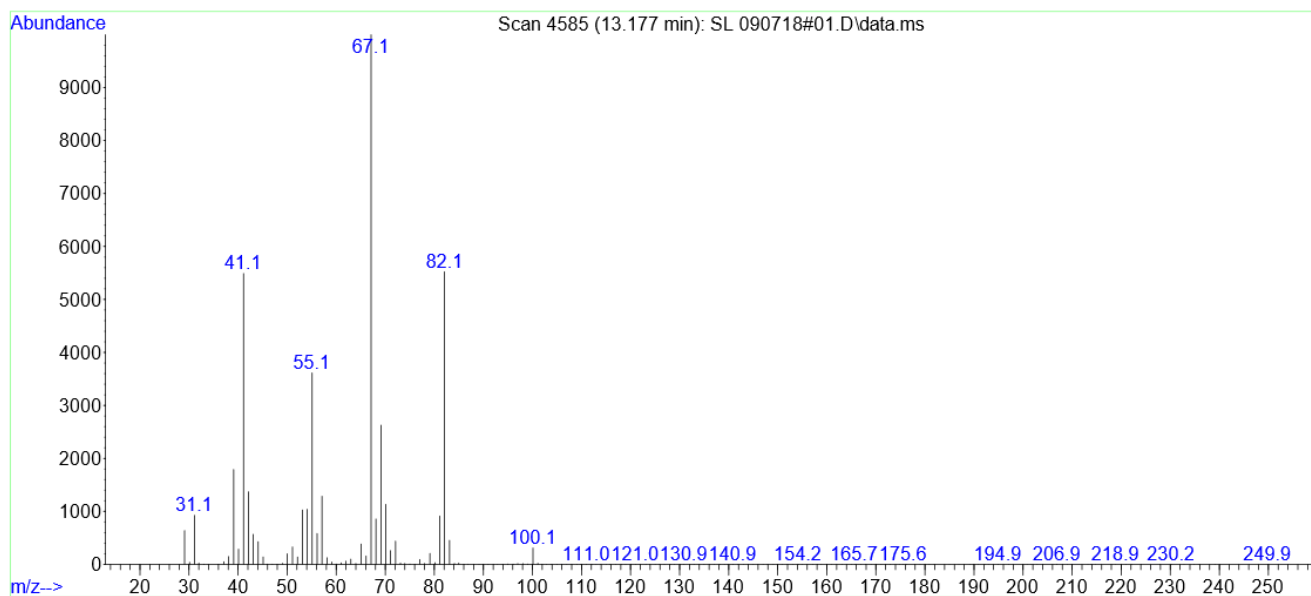
### 31. (Z)-3-hexen-1-ol



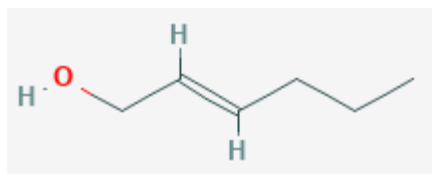
Library Searched : C:\Database\NIST11.L

Quality : 91

ID : 3-Hexen-1-ol, (Z)-



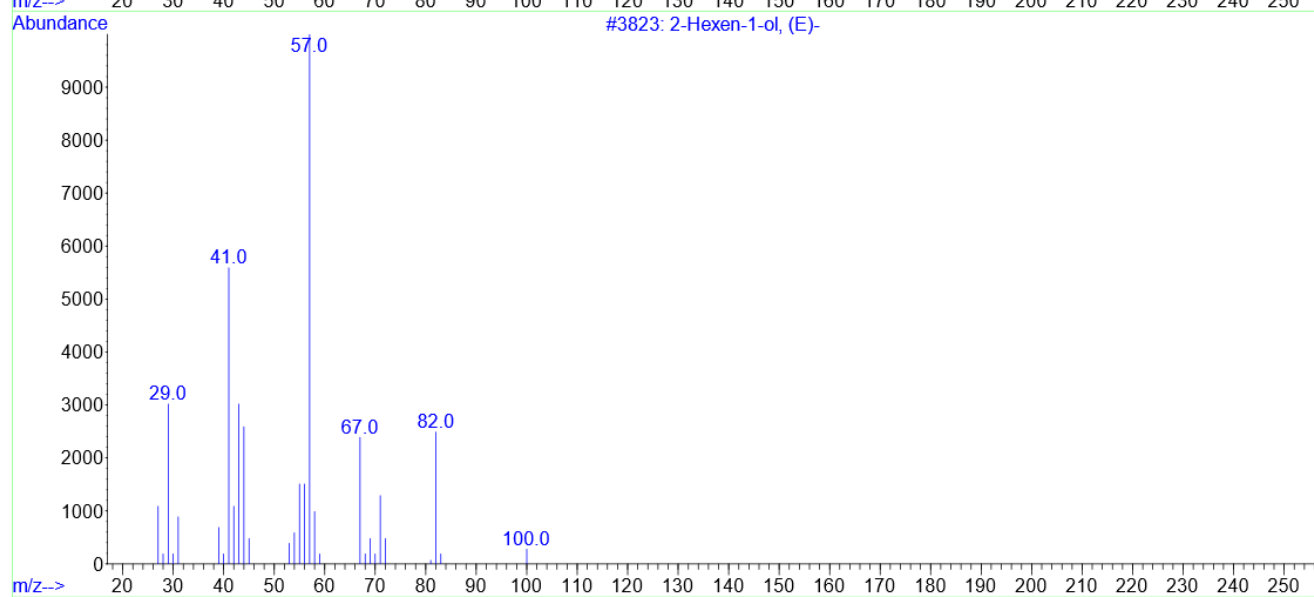
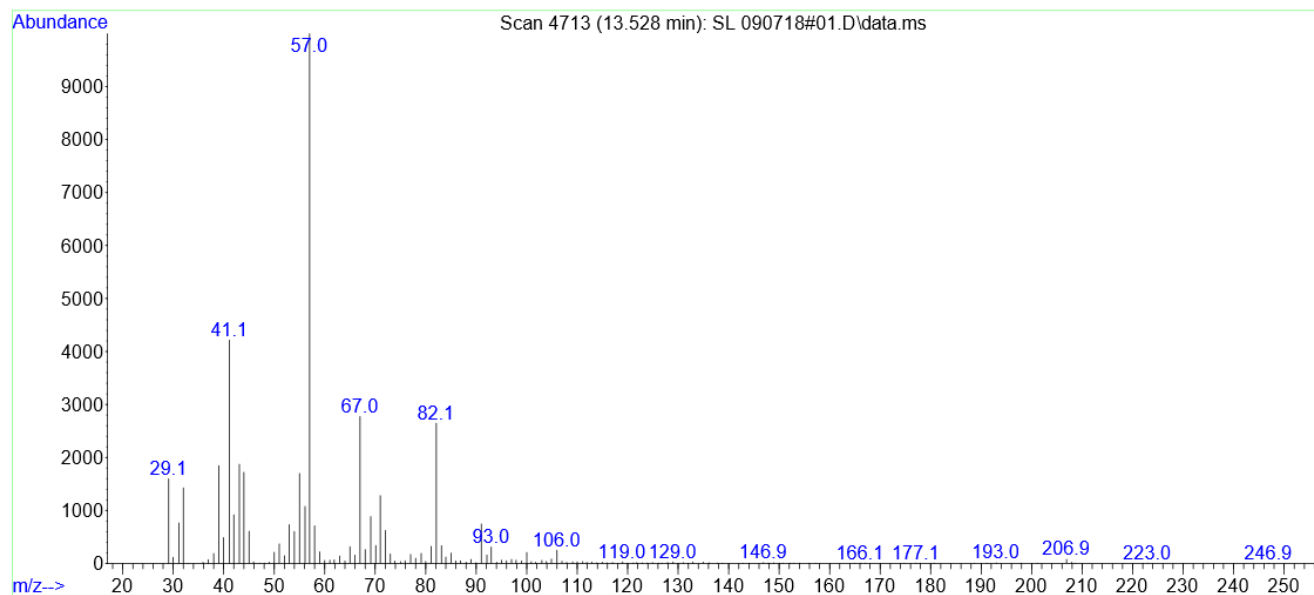
## 32. 2-hexen-1-ol



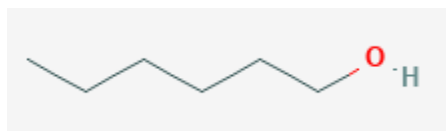
Library Searched : C:\Database\NIST11.L

Quality : 91

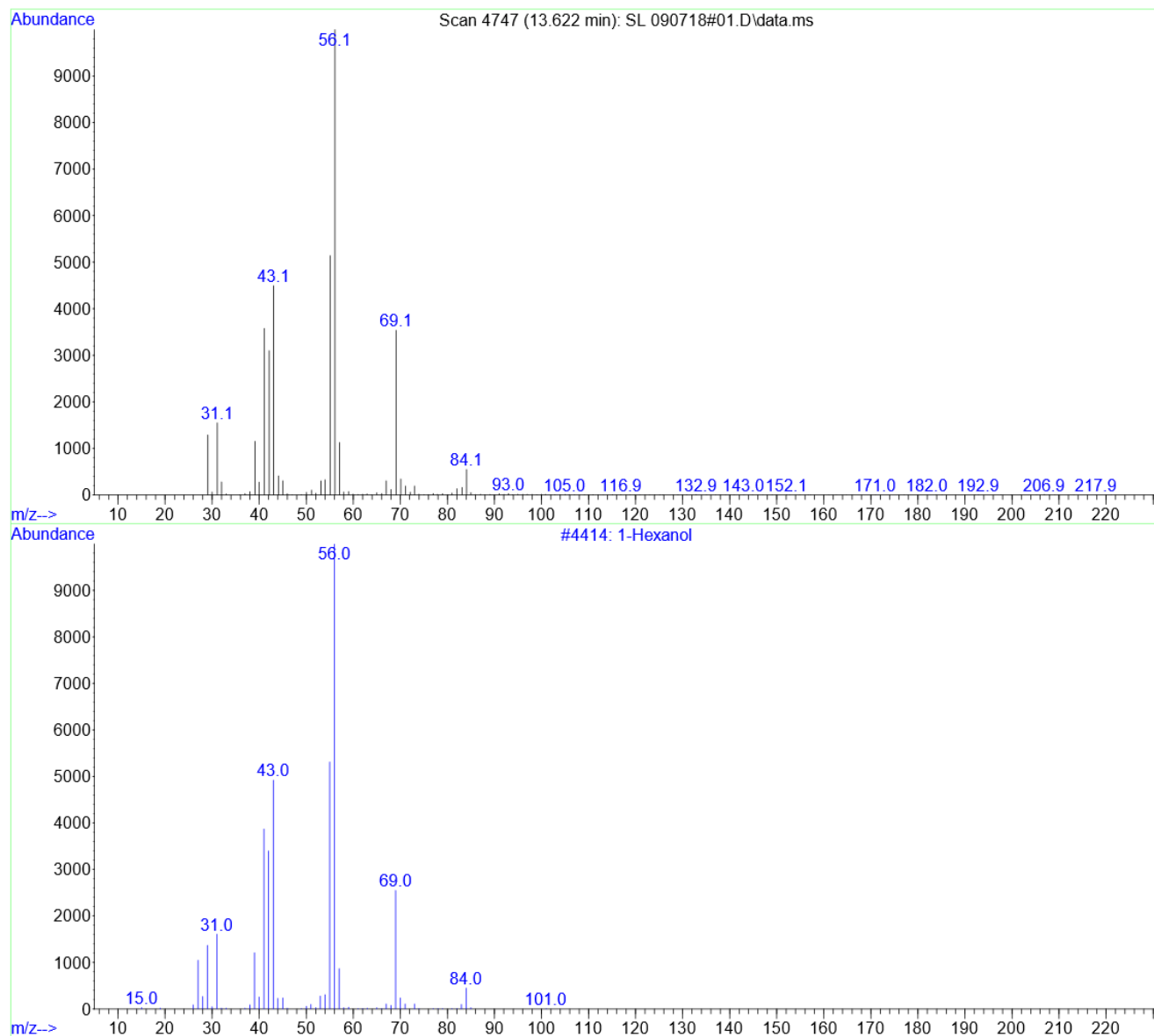
ID : 2-Hexen-1-ol, (E)-



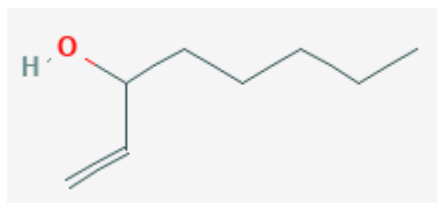
### 33. Hexan-1-ol



Library Searched : C:\Database\NIST11.L  
Quality : 90  
ID : 1-Hexanol



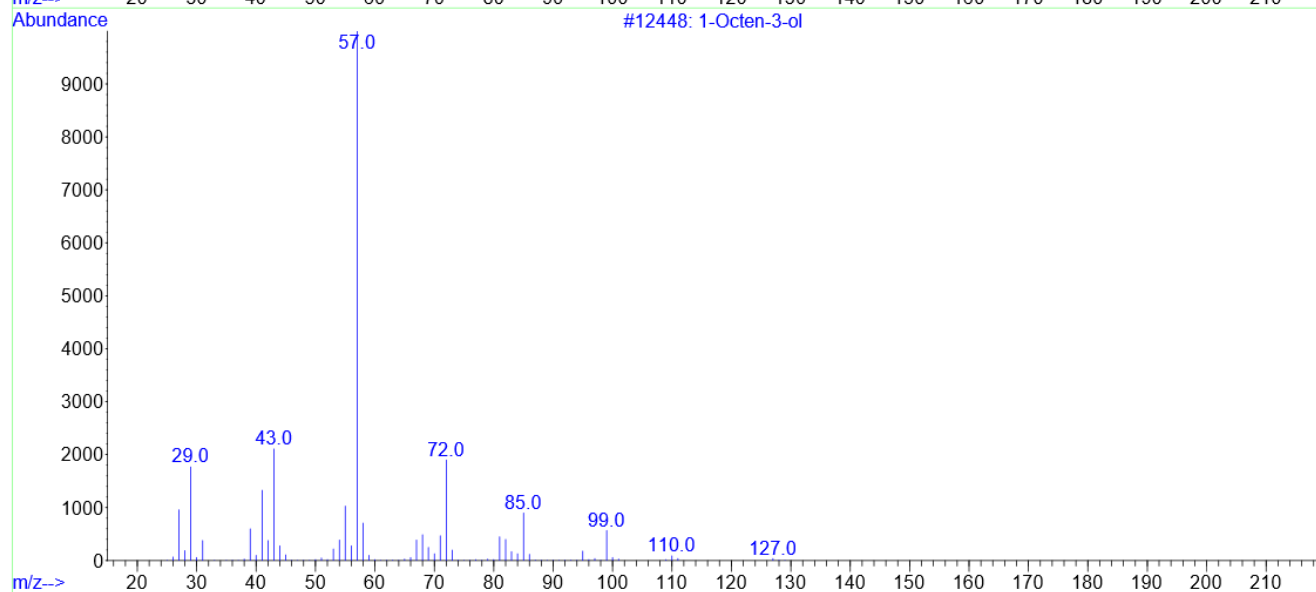
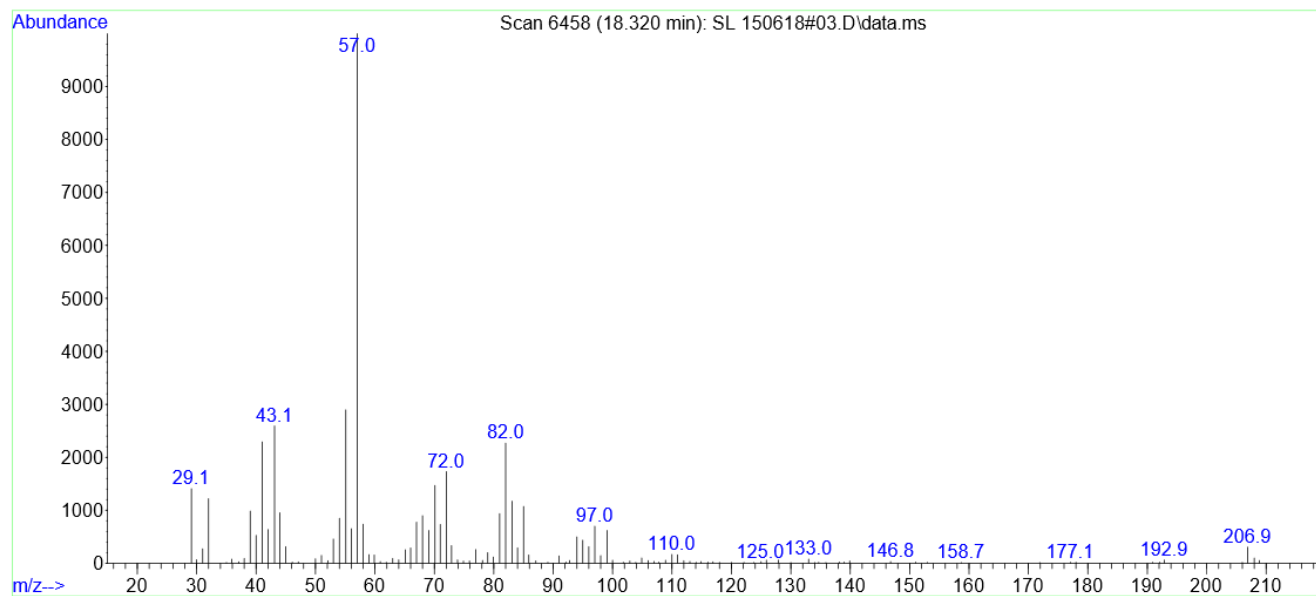
### 34. 1-octen-3-ol



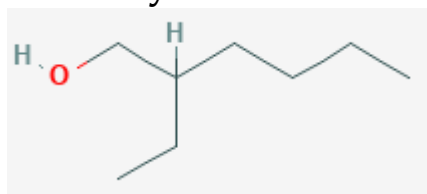
Library Searched : C:\Database\NIST11.L

Quality : 47

ID : 1-Octen-3-ol



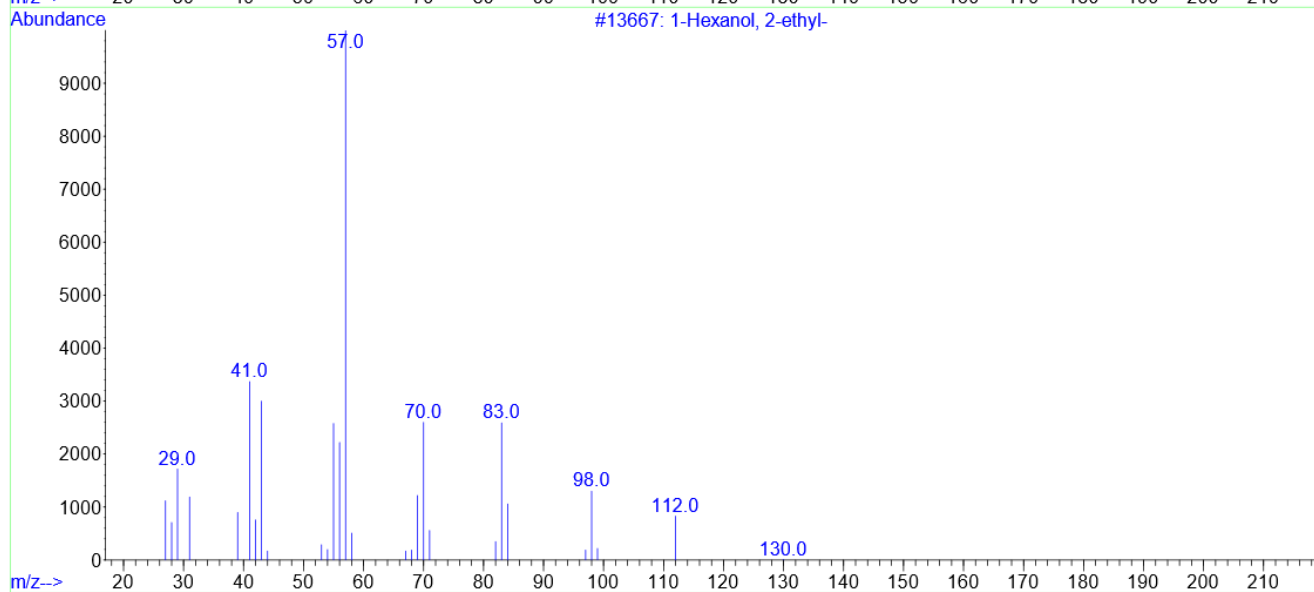
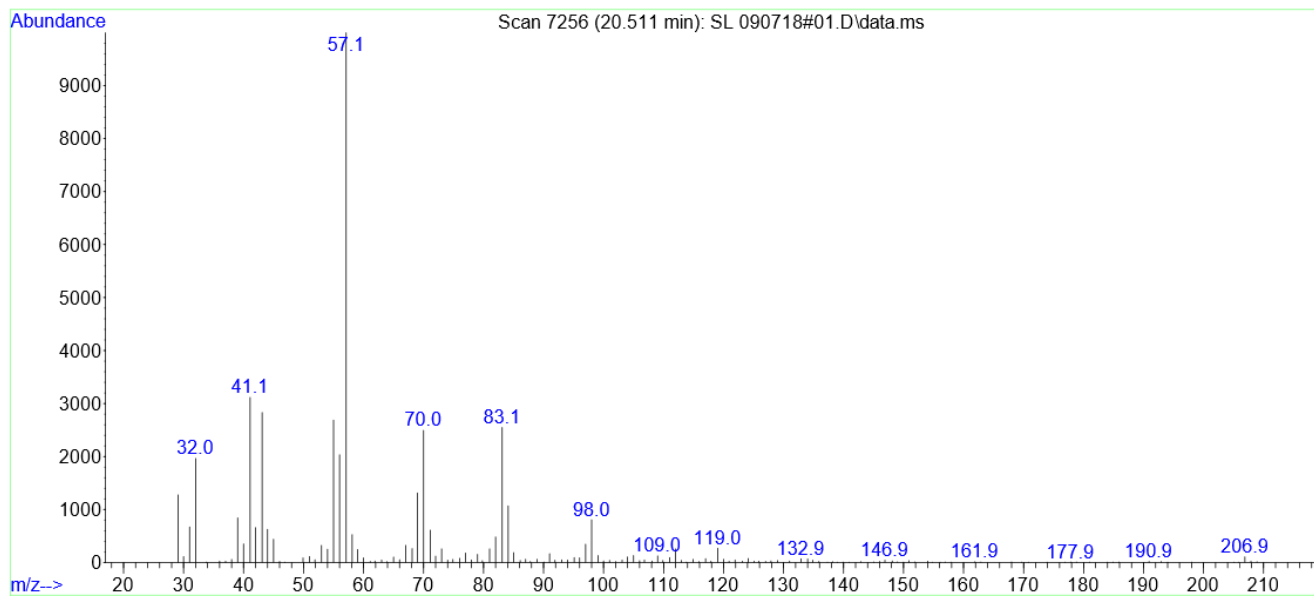
## 35. 2-ethylhexanol



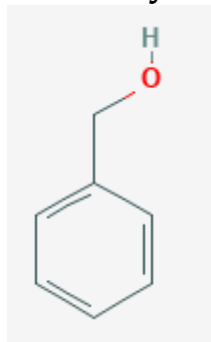
Library Searched : C:\Database\NIST11.L

Quality : 86

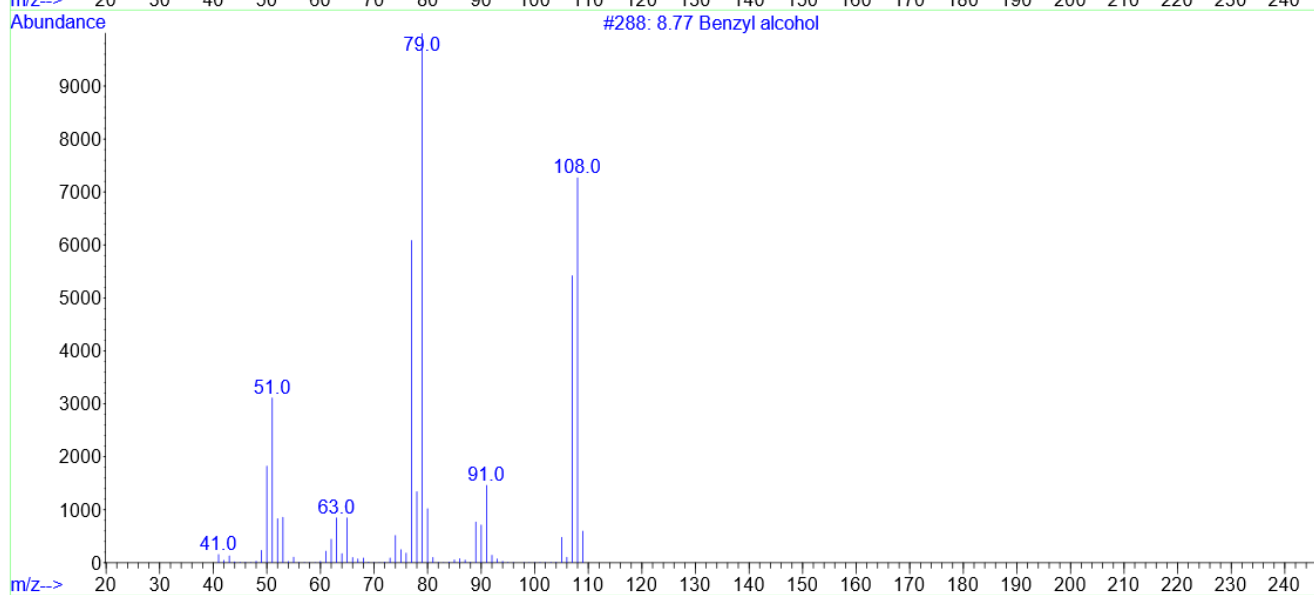
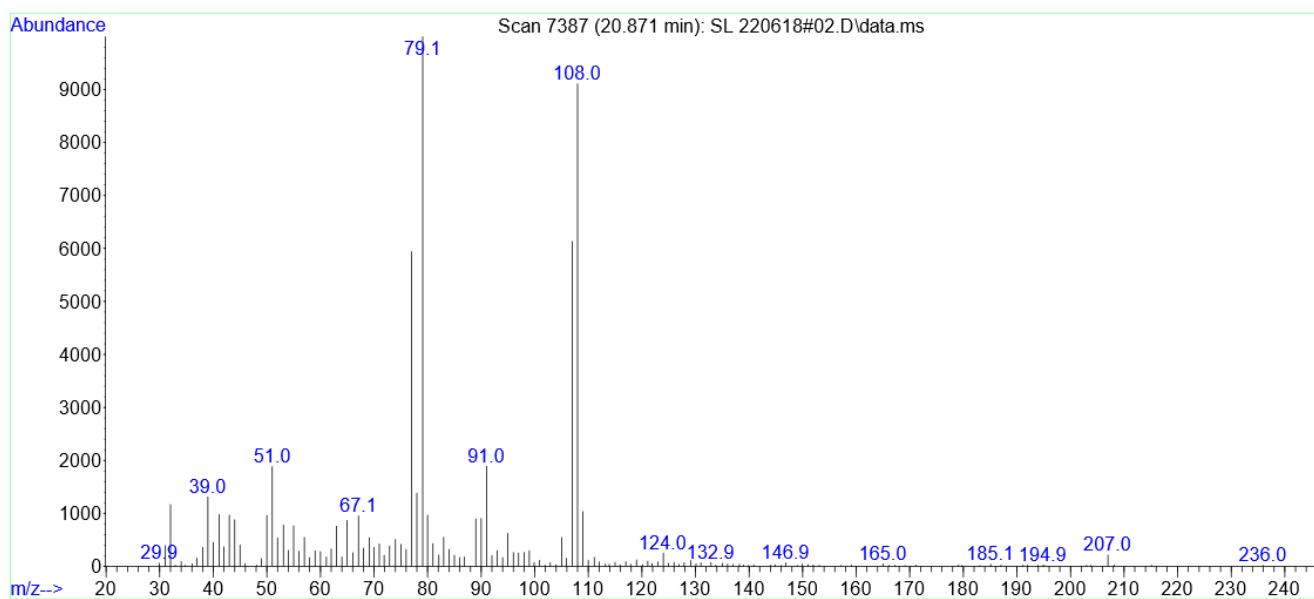
ID : 1-Hexanol, 2-ethyl-



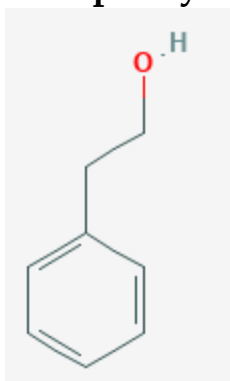
### 36. Benzyl alcohol



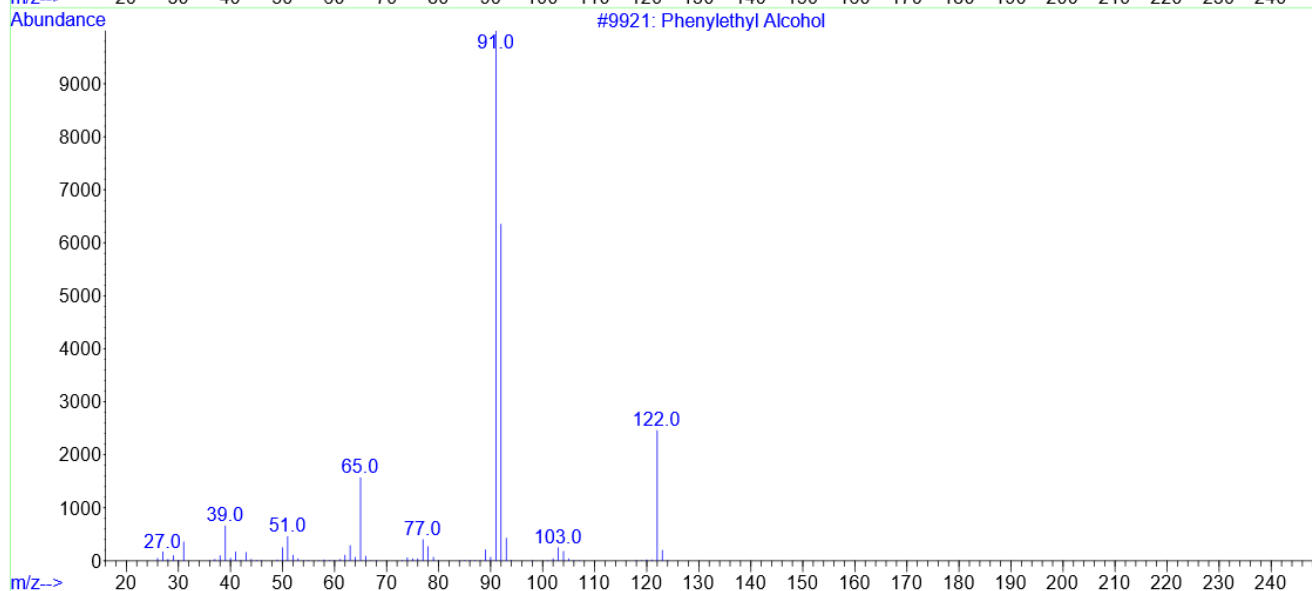
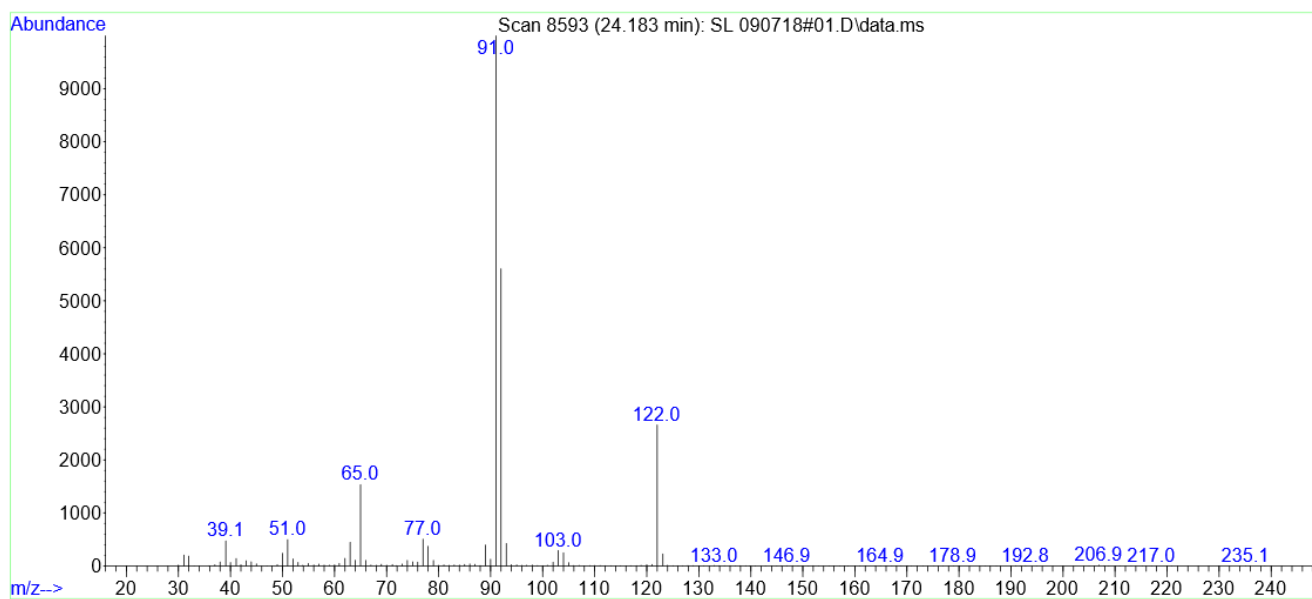
Library Searched : C:\Database\Adams.L  
Quality : 97  
ID : 8.77 Benzyl alcohol



## 37. 2-phenylethanol



Library Searched : C:\Database\NIST11.L  
Quality : 94  
ID : Phenylethyl Alcohol



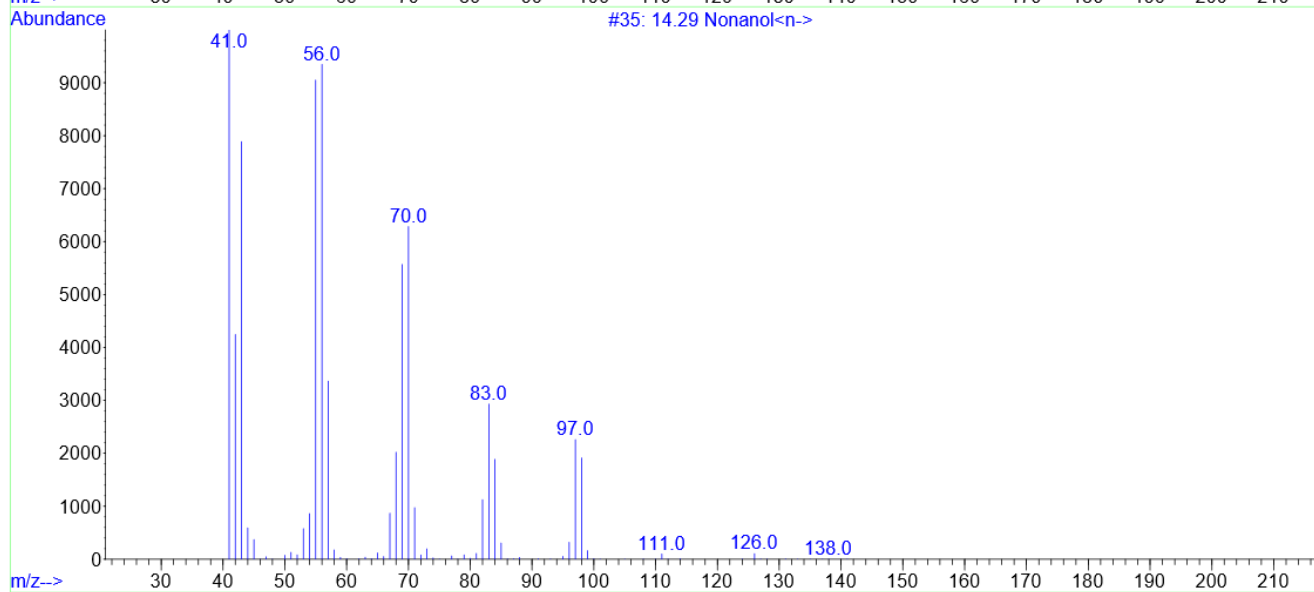
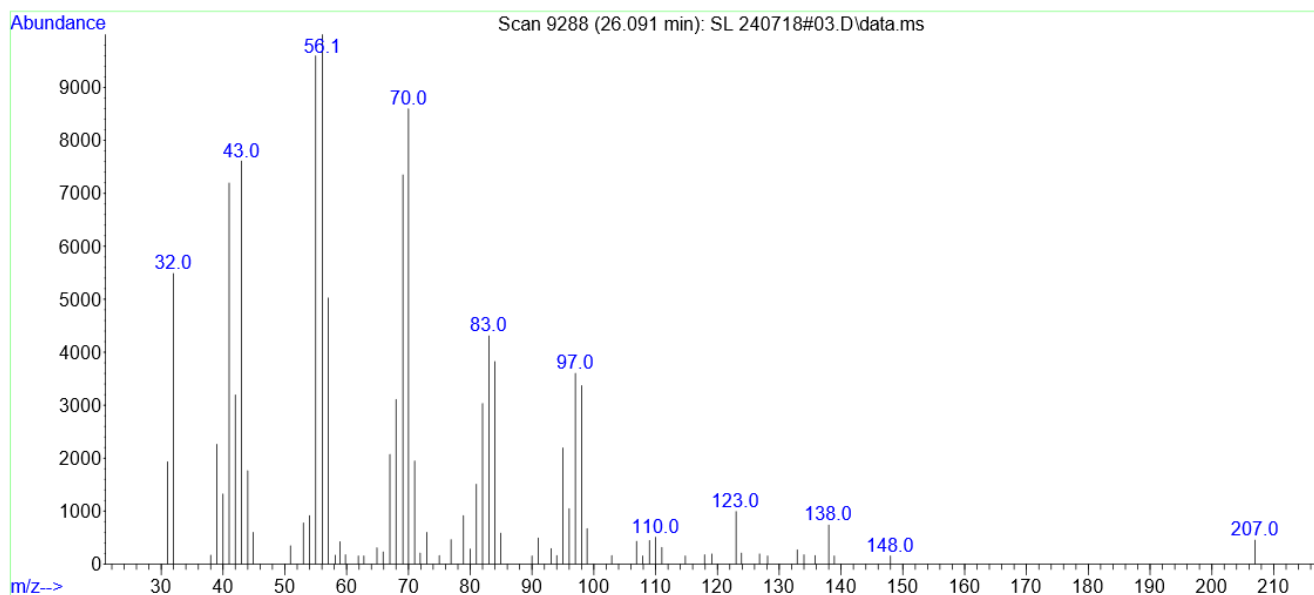
### 38. 1-nonanol



Library Searched : C:\Database\Adams.L

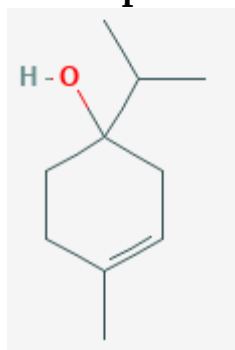
Quality : 78

ID : 14.29 Nonanol<n->





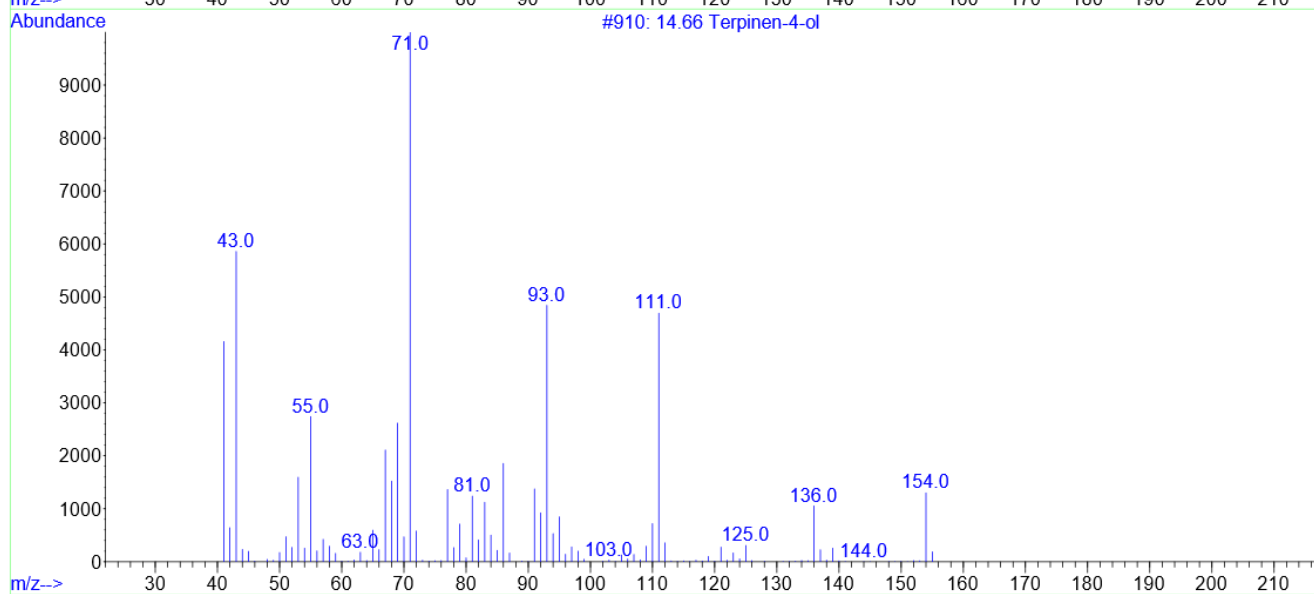
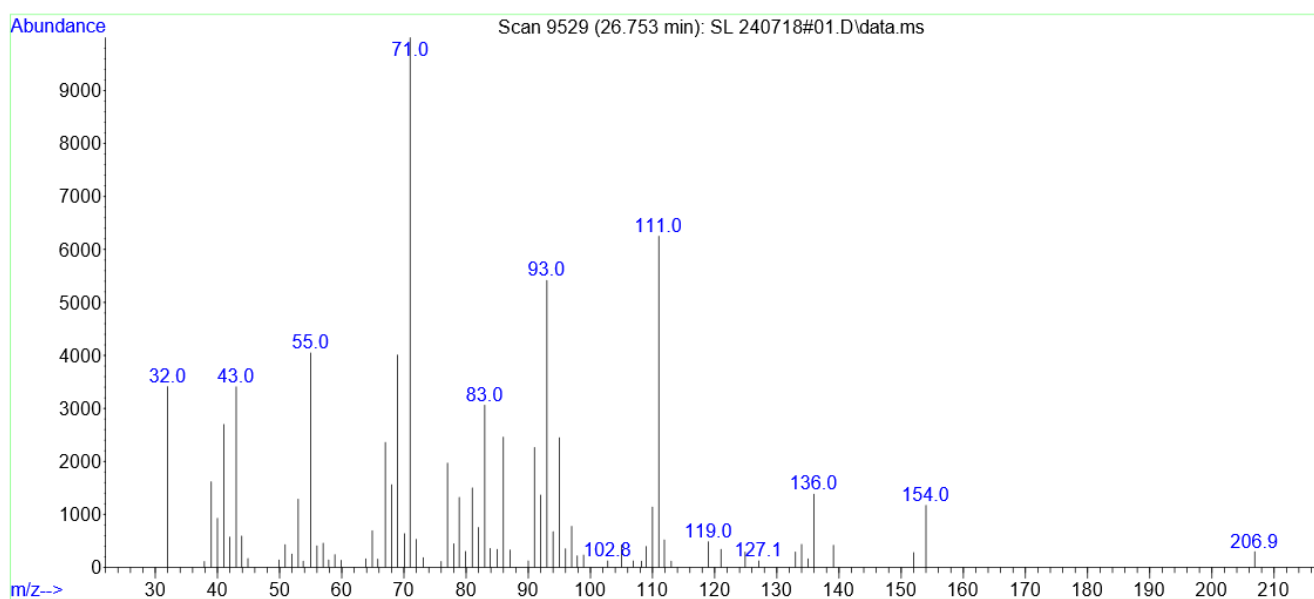
### 39. Terpinen-4-ol



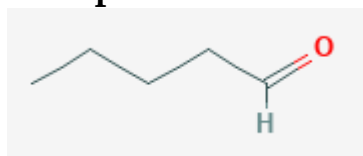
Library Searched : C:\Database\Adams.L

Quality : 93

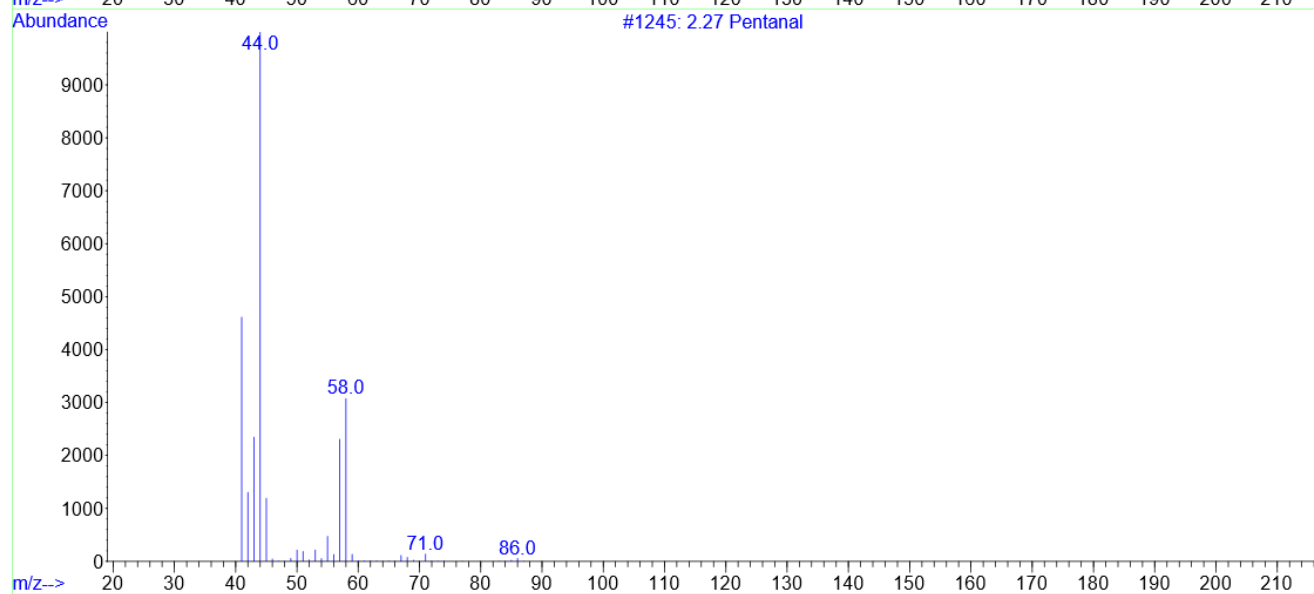
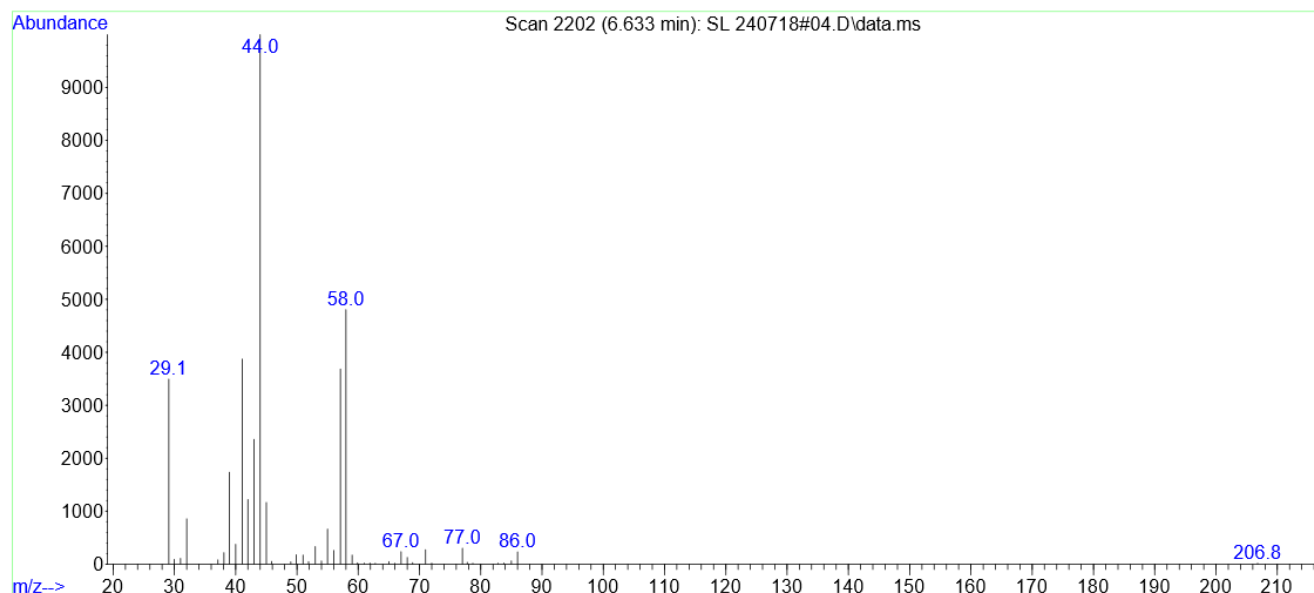
ID : 14.66 Terpinen-4-ol



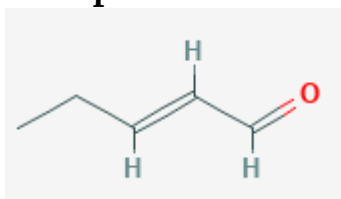
## 40. 2-pentanal



Library Searched : C:\Database\Adams.L  
Quality : 87  
ID : 2.27 Pentanal



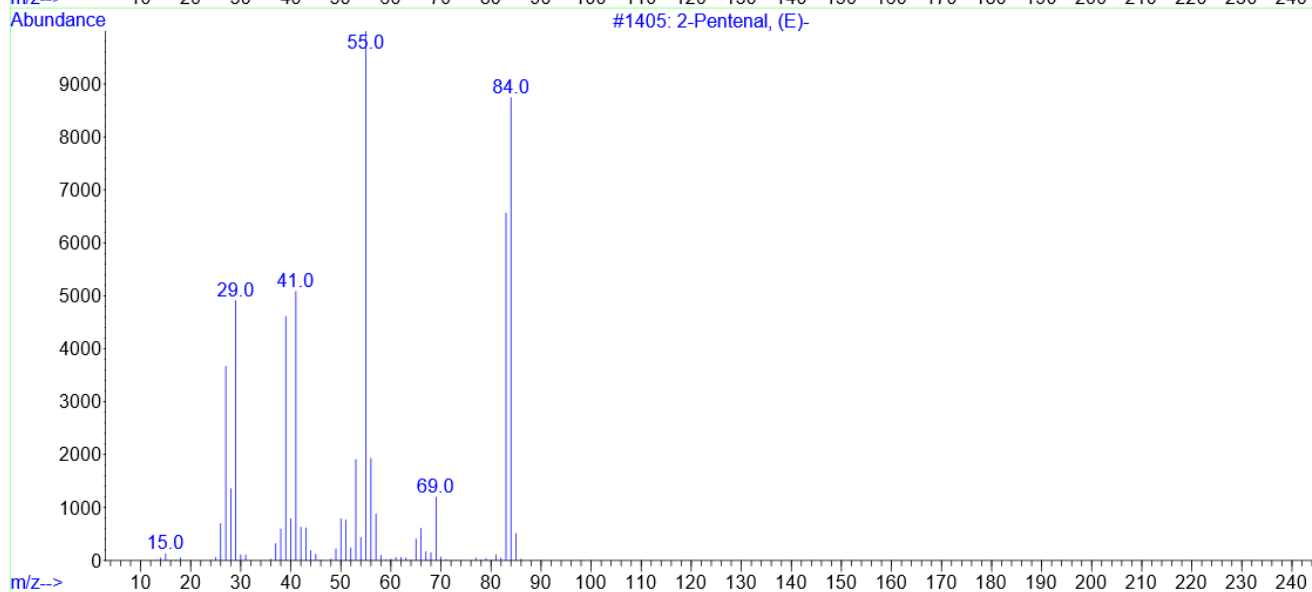
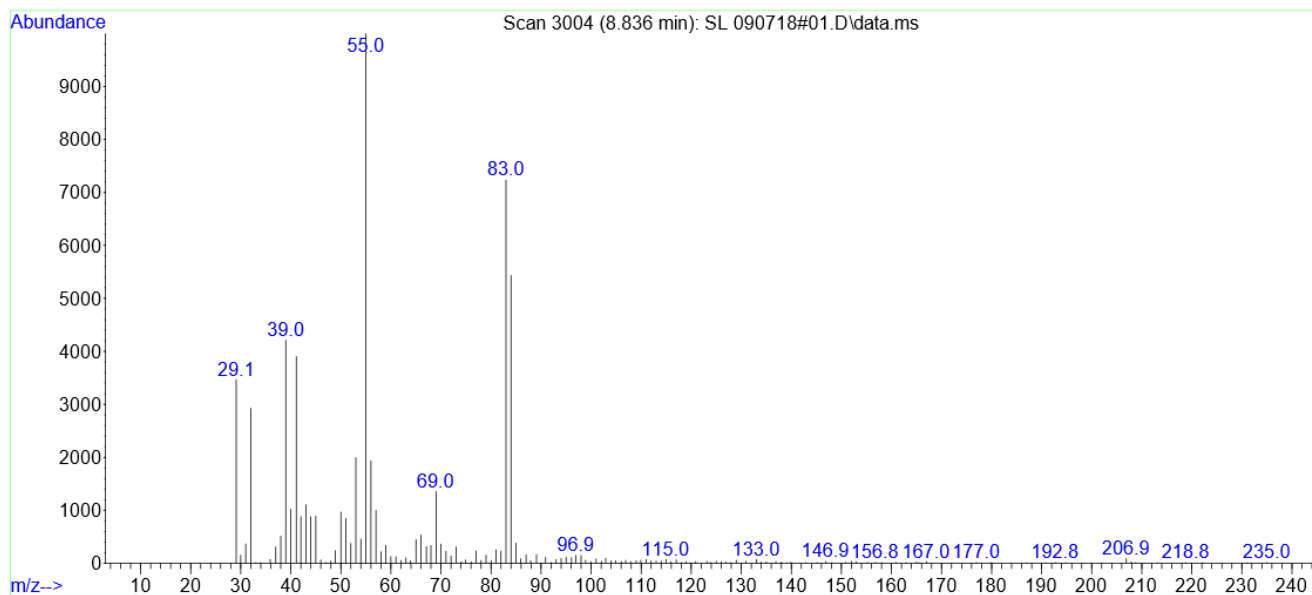
## 41. 2-pentenal



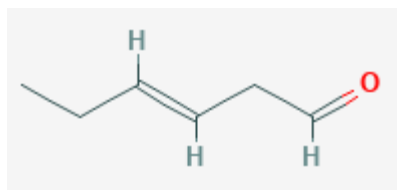
Library Searched : C:\Database\NIST11.L

Quality : 81

ID : 2-Pentenal, (E)-



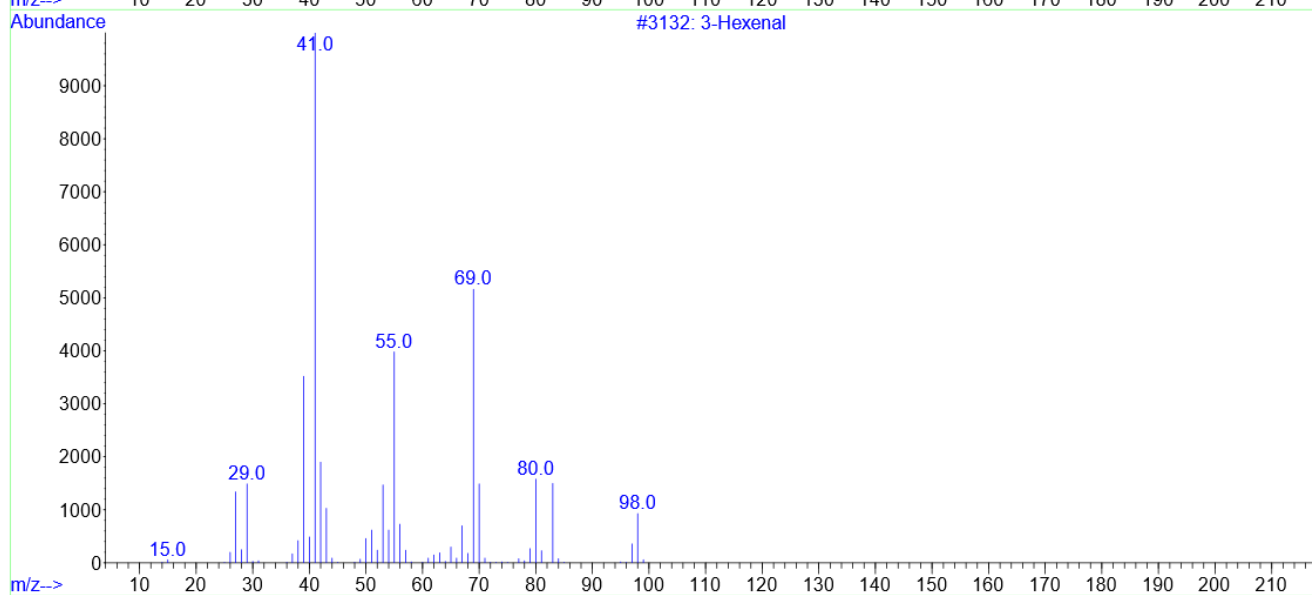
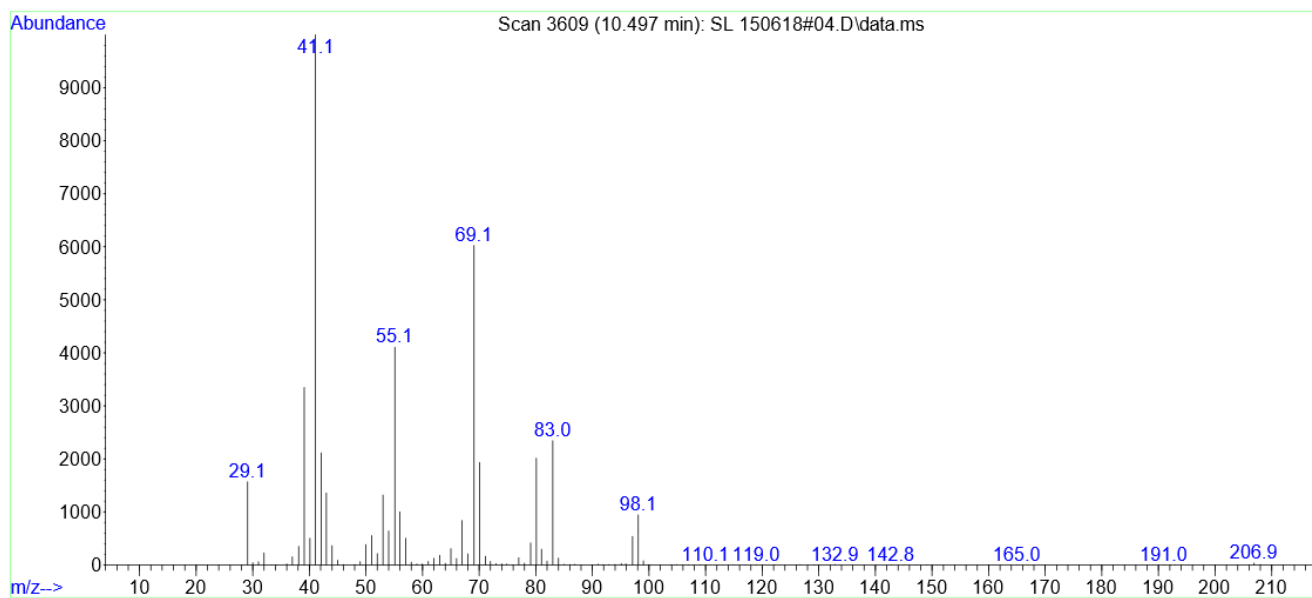
## 42. 3-hexenal



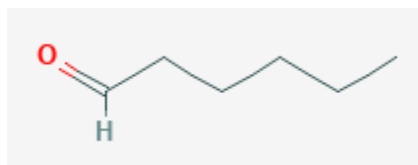
Library Searched : C:\Database\NIST11.L

Quality : 90

ID : 3-Hexenal



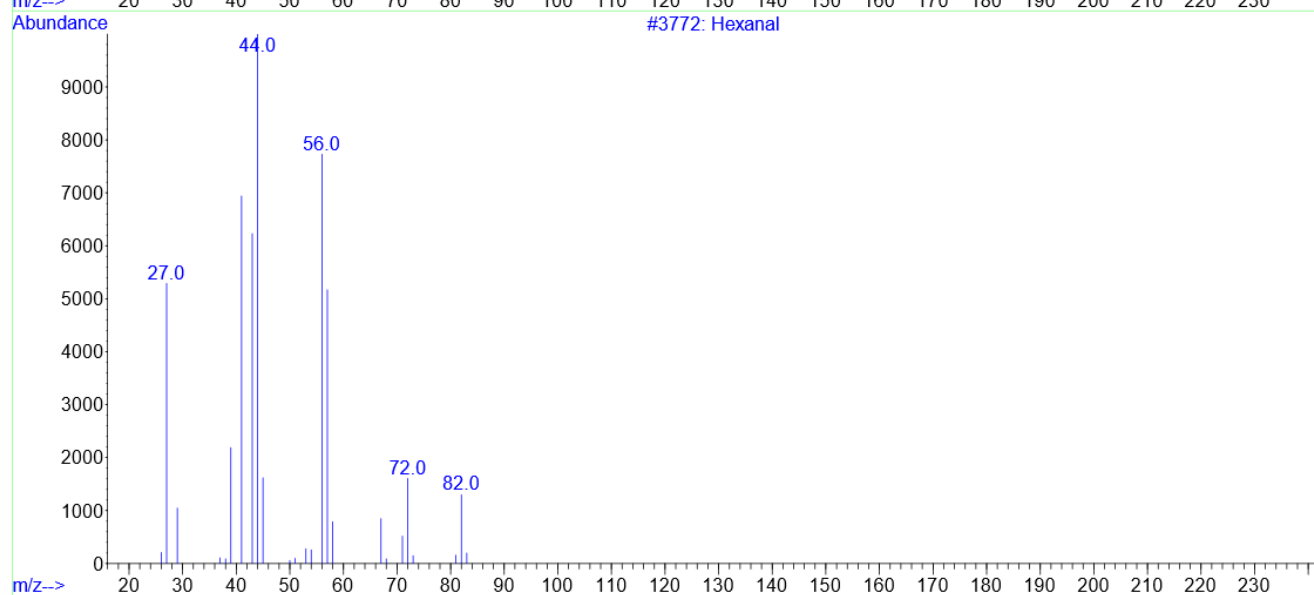
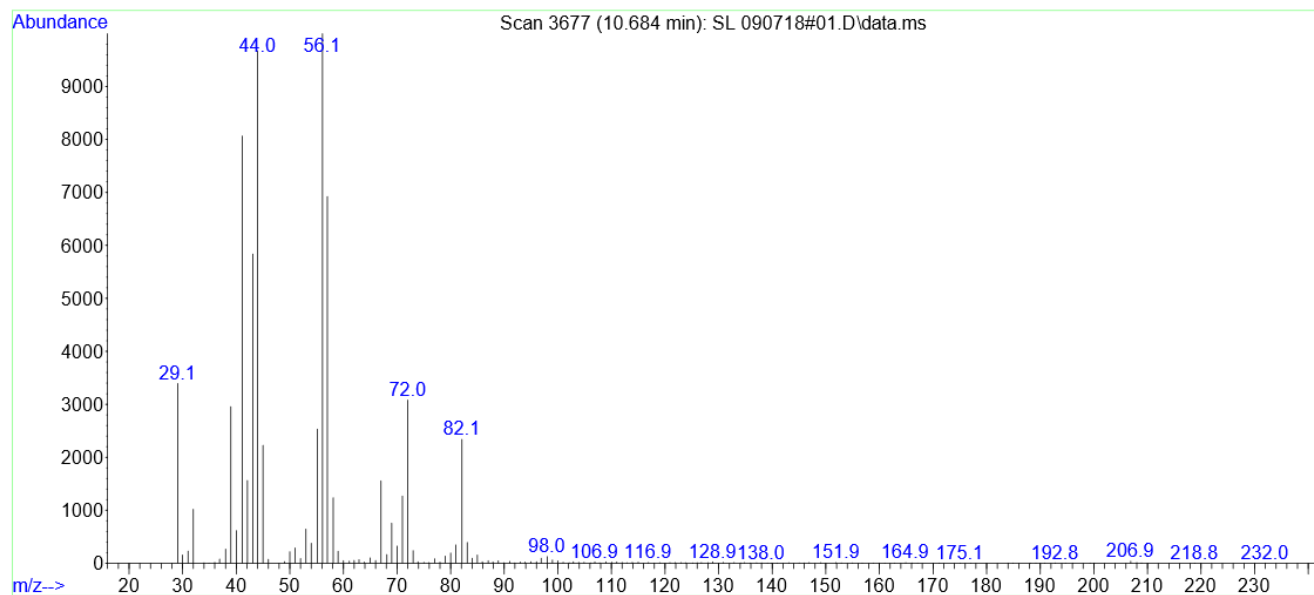
## 43. Hexanal



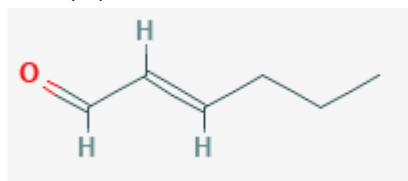
Library Searched : C:\Database\NIST11.L

Quality : 90

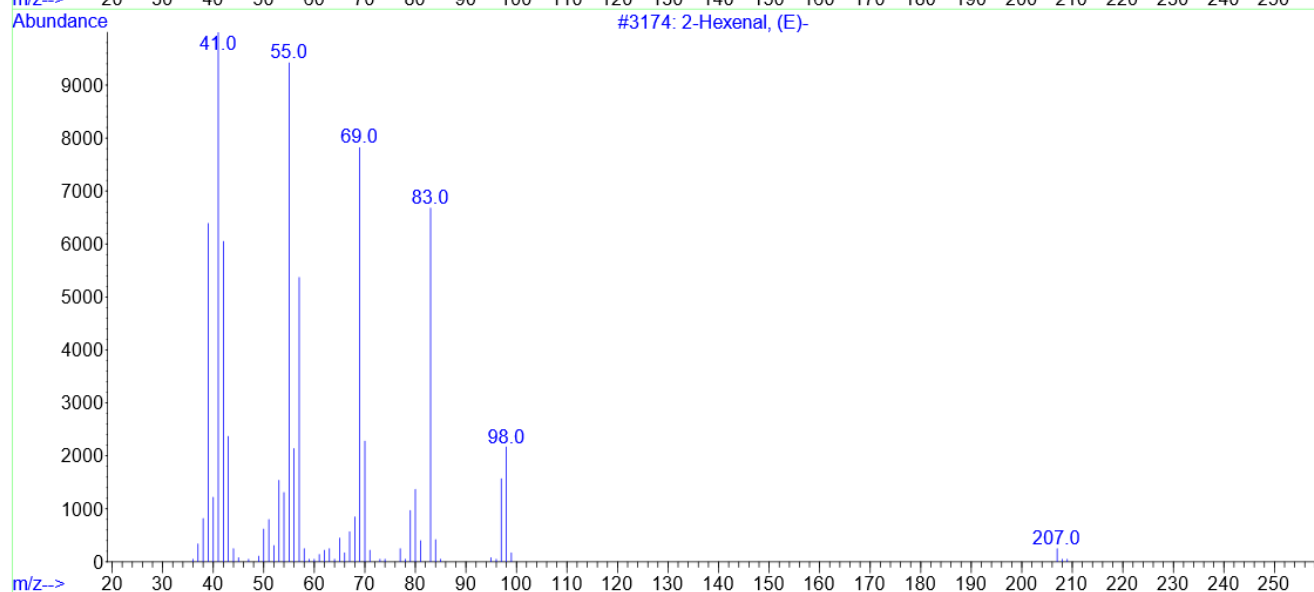
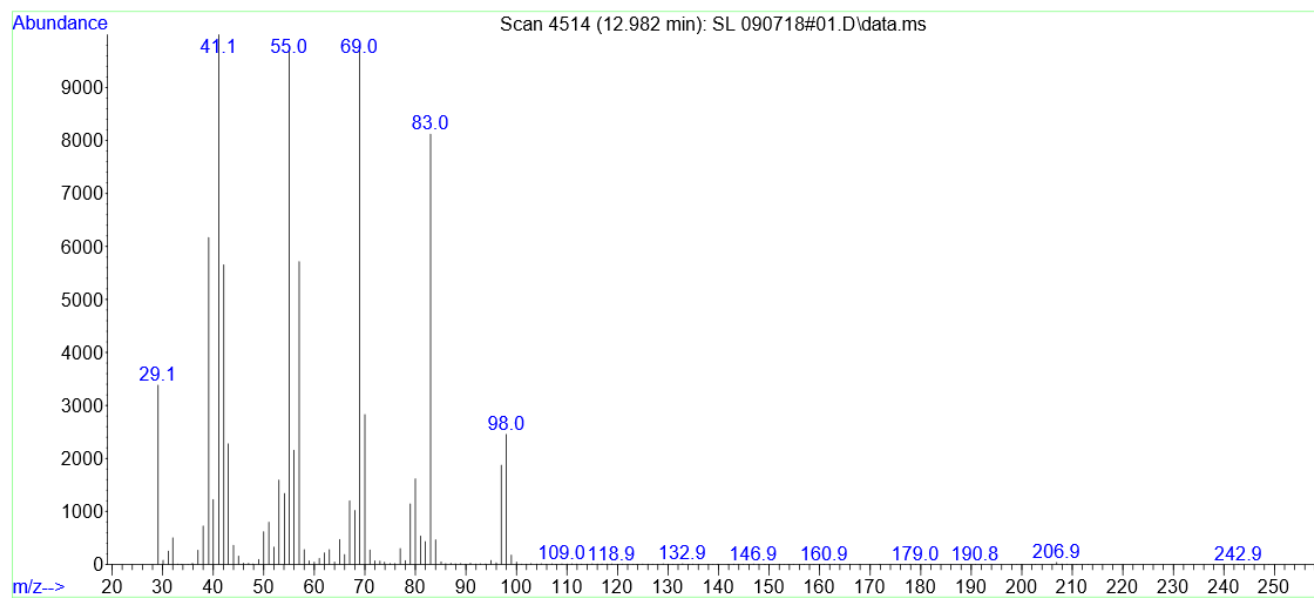
ID : Hexanal



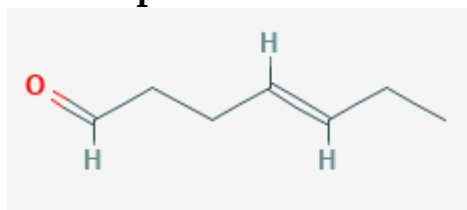
## 44. (E)-2-hexenal



Library Searched : C:\Database\NIST11.L  
Quality : 98  
ID : 2-Hexenal, (E)-



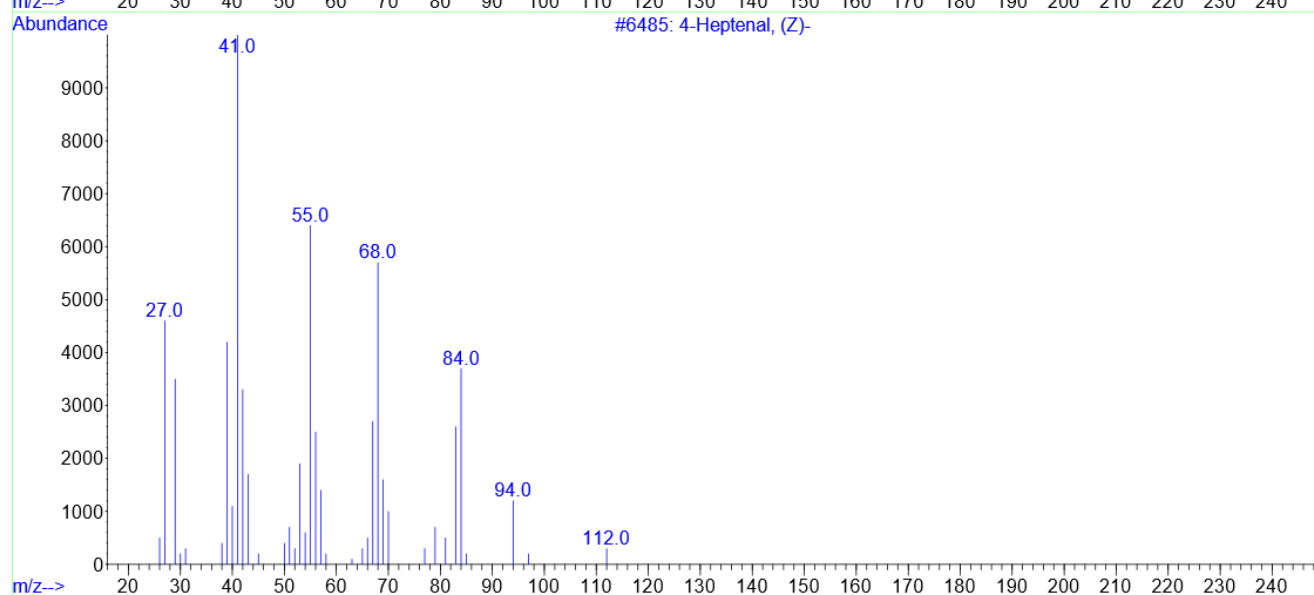
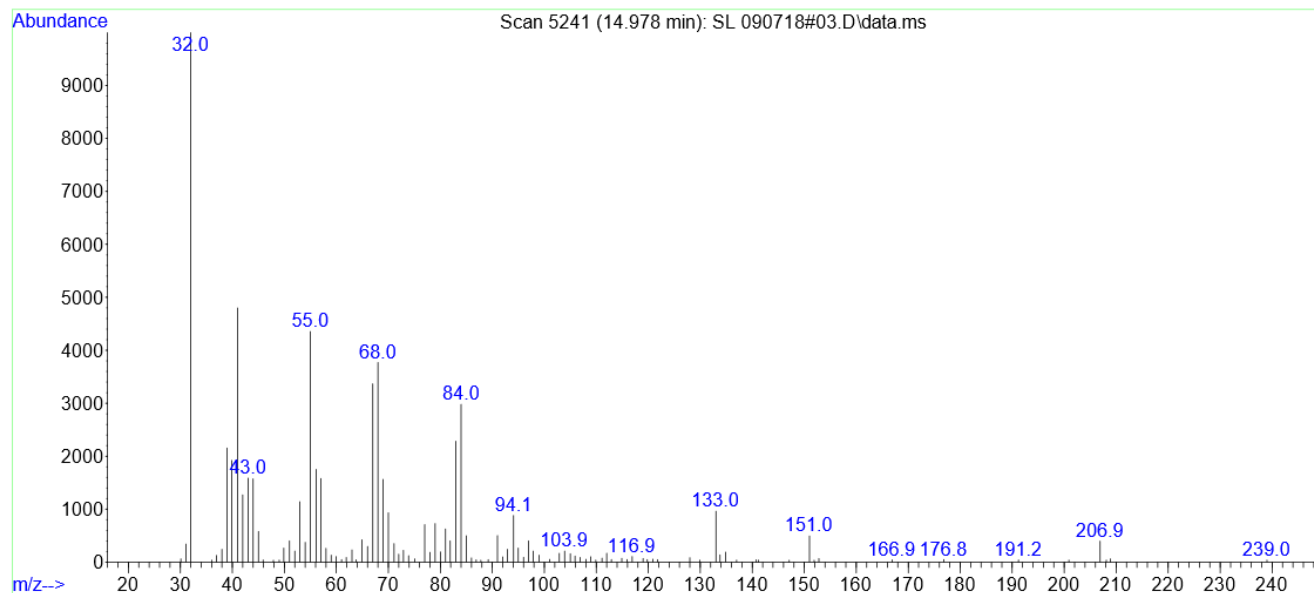
## 45. 4-heptenal



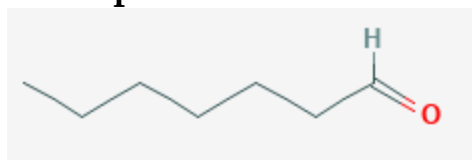
Library Searched : C:\Database\NIST11.L

Quality : 50

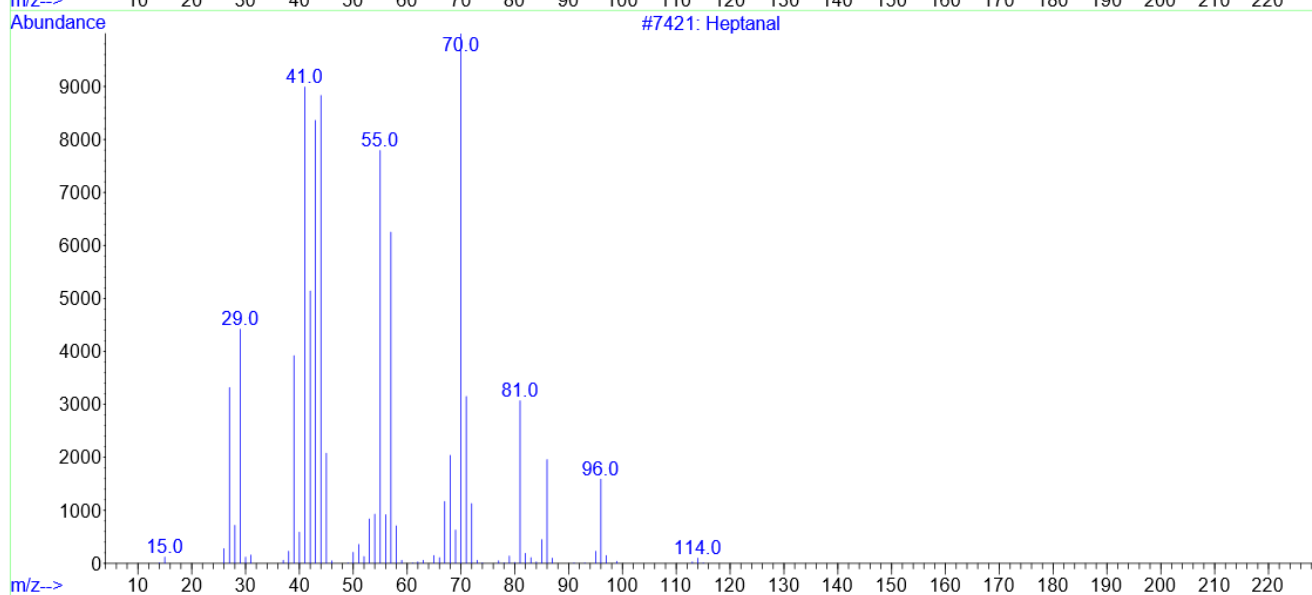
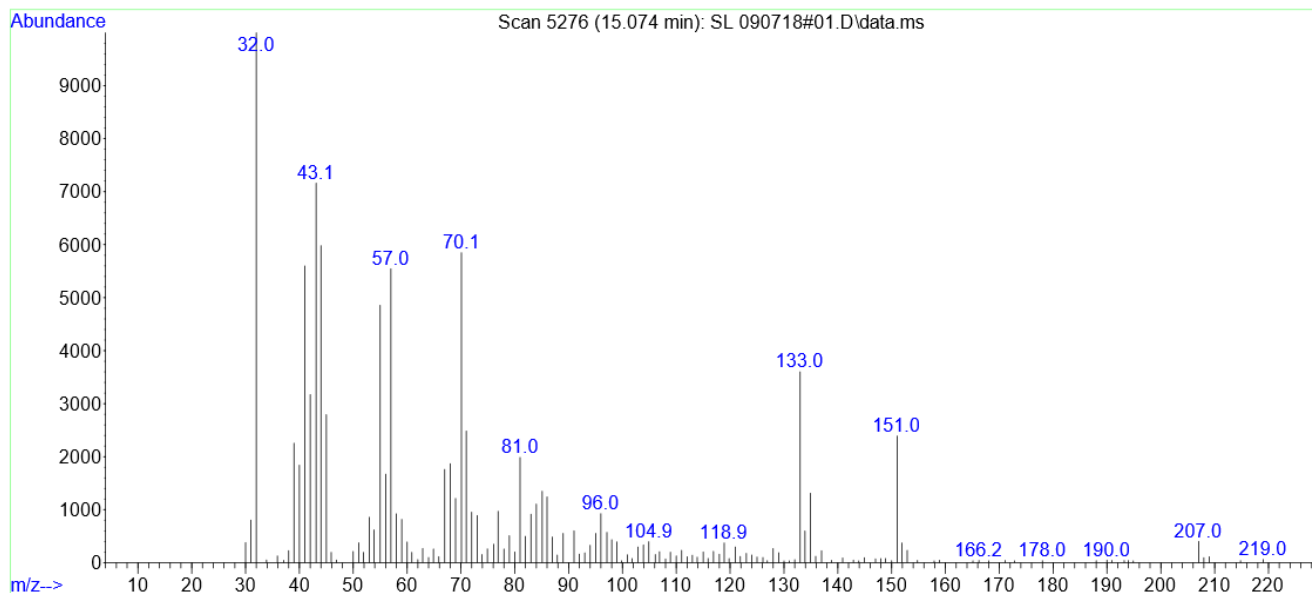
ID : 4-Heptenal, (Z)-



## 46. Heptanal

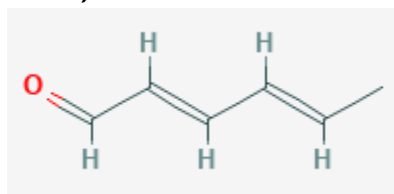


Library Searched : C:\Database\NIST11.L  
Quality : 92  
ID : Heptanal





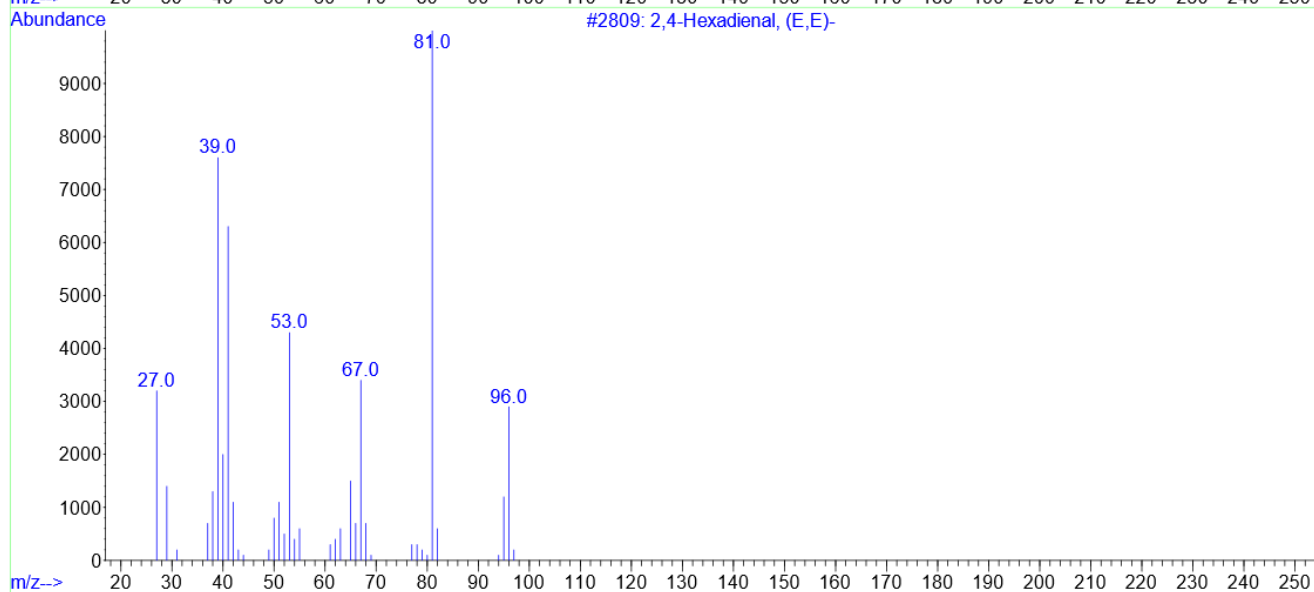
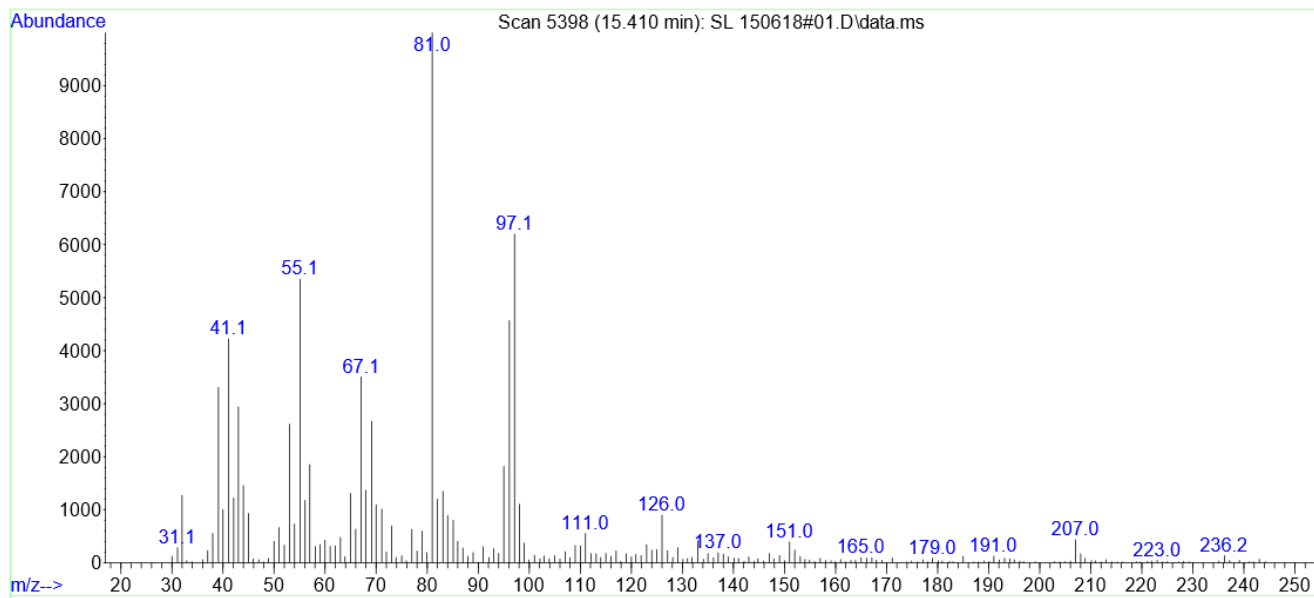
## 47. 2,4-hexadienal



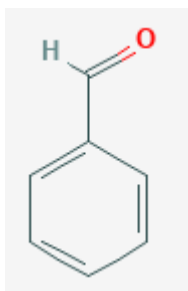
Library Searched : C:\Database\NIST11.L

Quality : 70

ID : 2,4-Hexadienal, (E,E)-



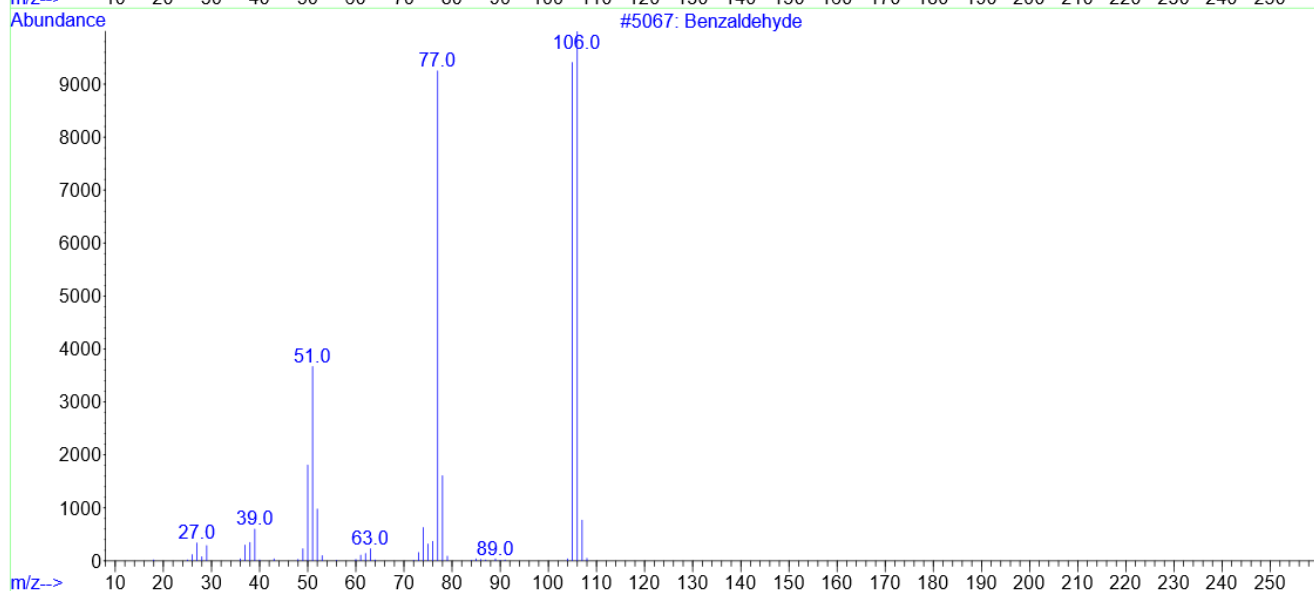
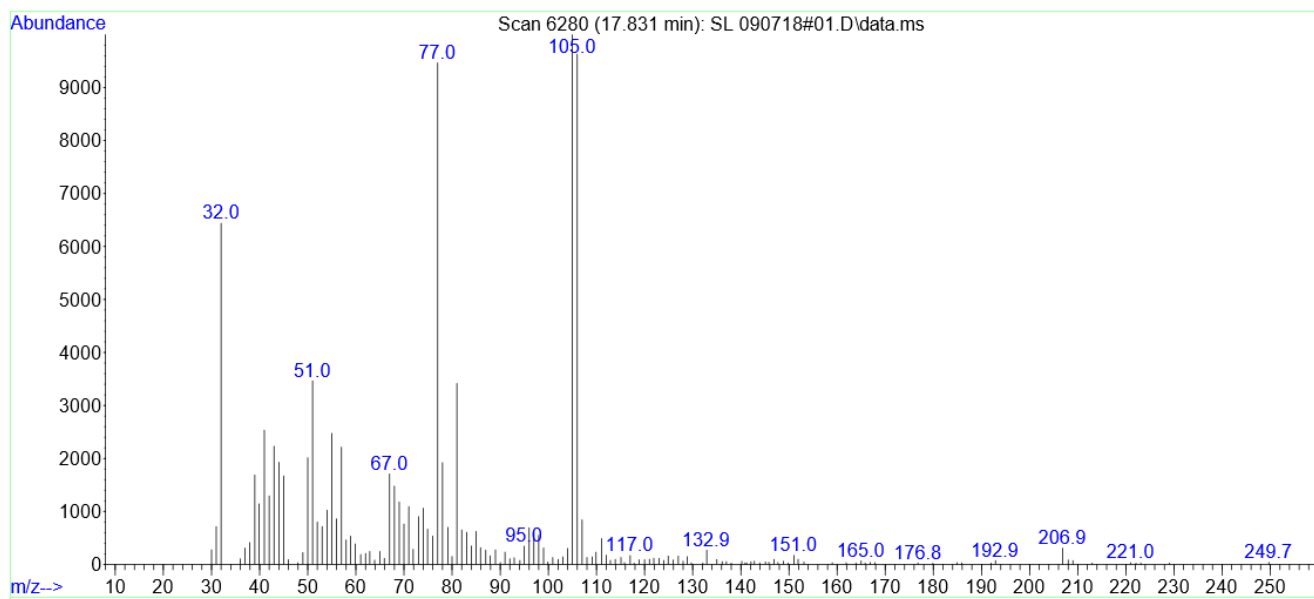
## 48. Benzaldehyde



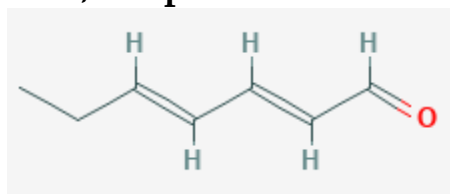
Library Searched : C:\Database\NIST11.L

Quality : 95

ID : Benzaldehyde



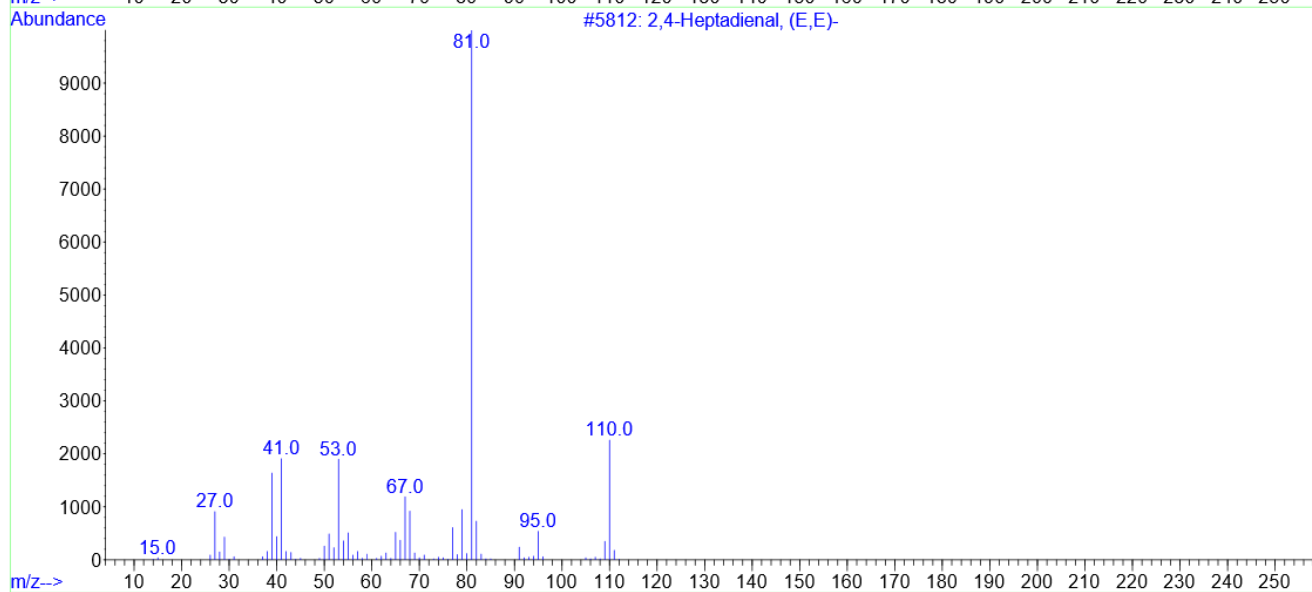
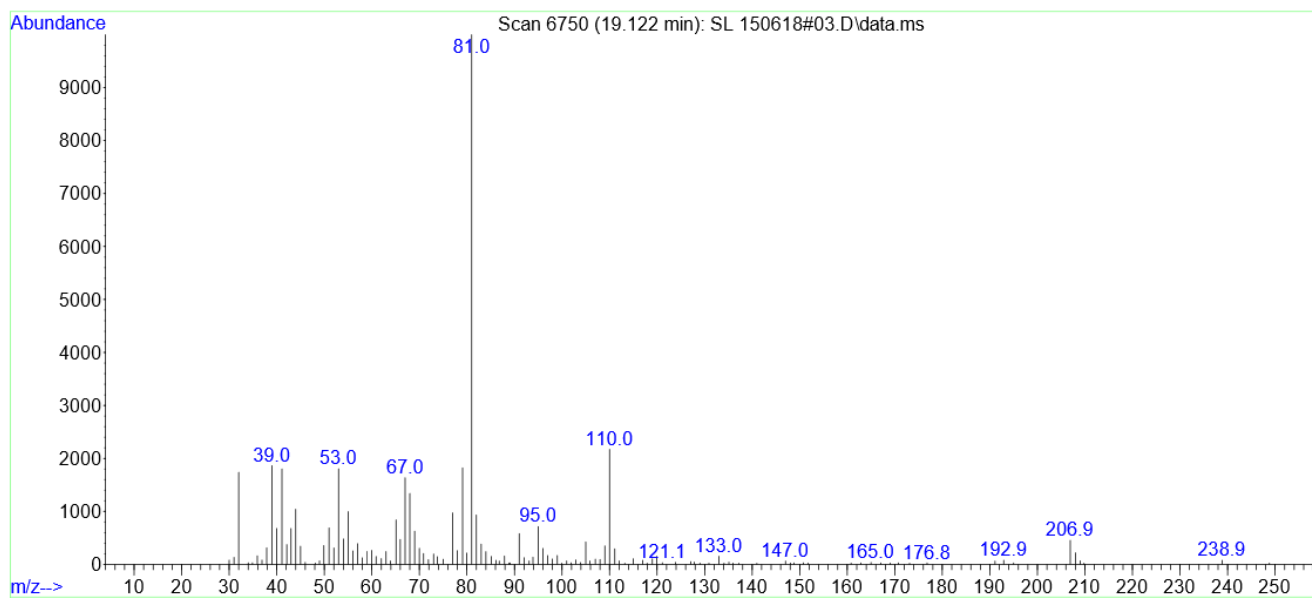
## 49. 2,4-heptadienal isomer 1



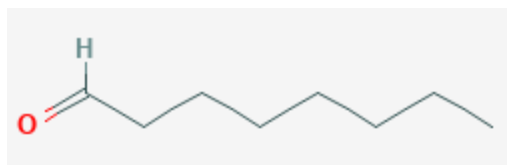
Library Searched : C:\Database\NIST11.L

Quality : 93

ID : 2,4-Heptadienal, (E,E)-



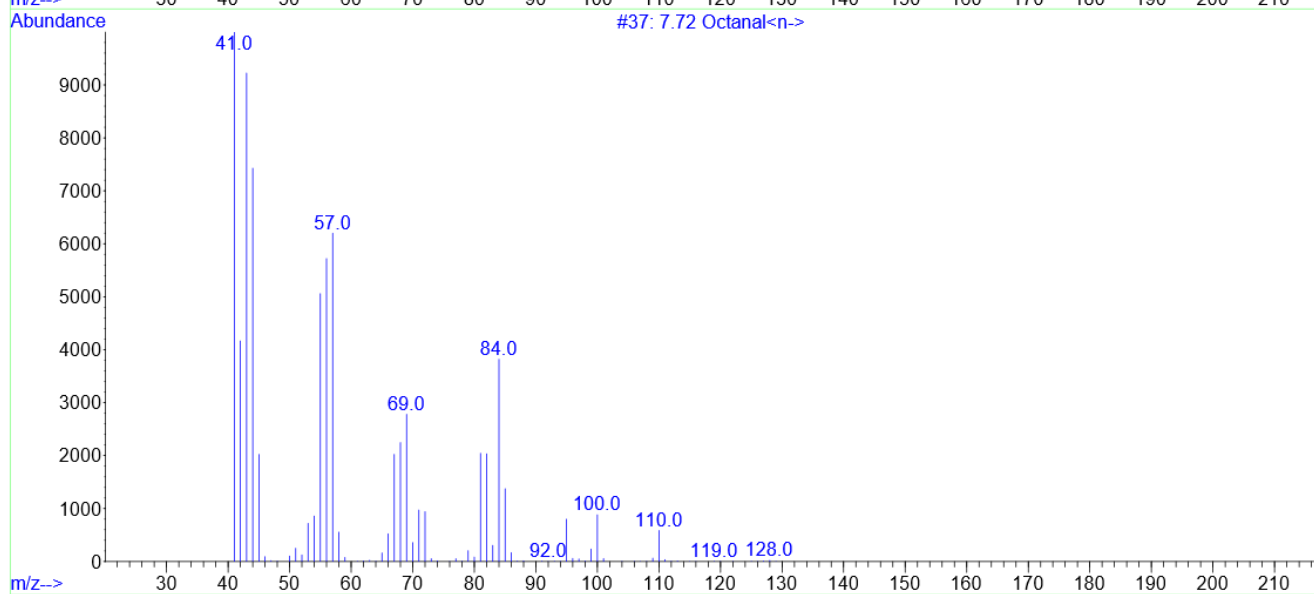
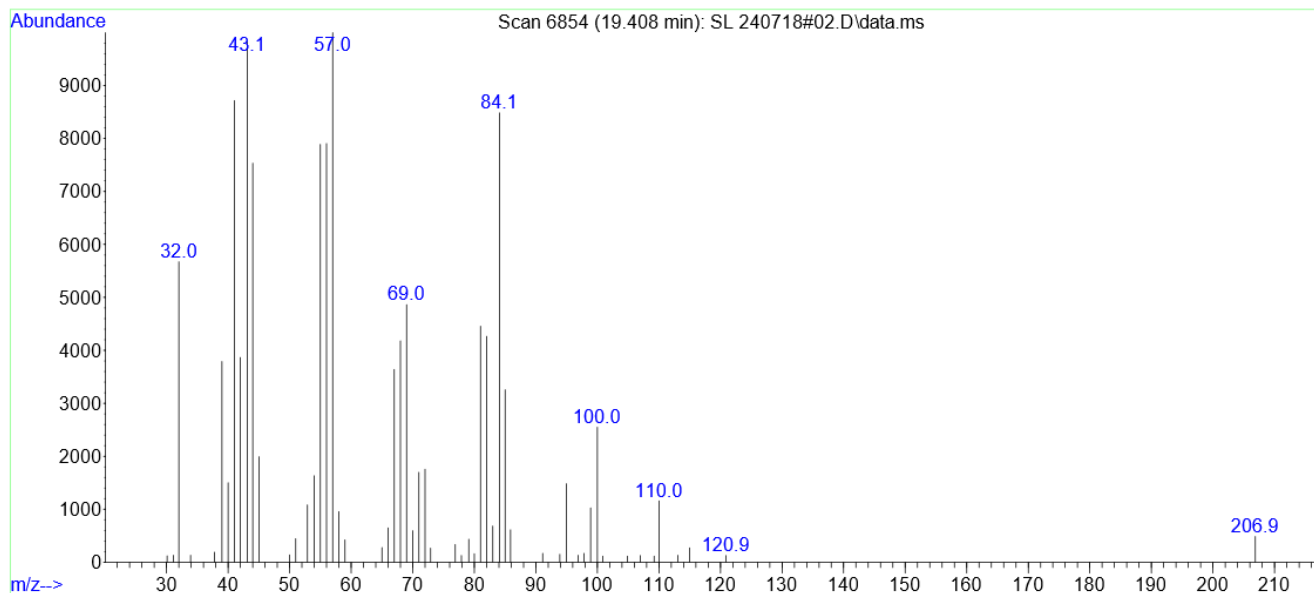
## 50. Octanal



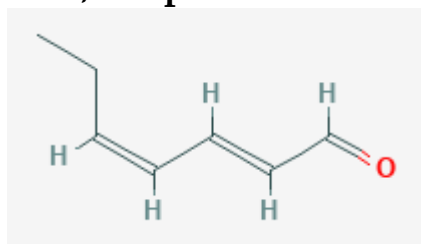
Library Searched : C:\Database\Adams.L

Quality : 90

ID : 7.72 Octanal<n->



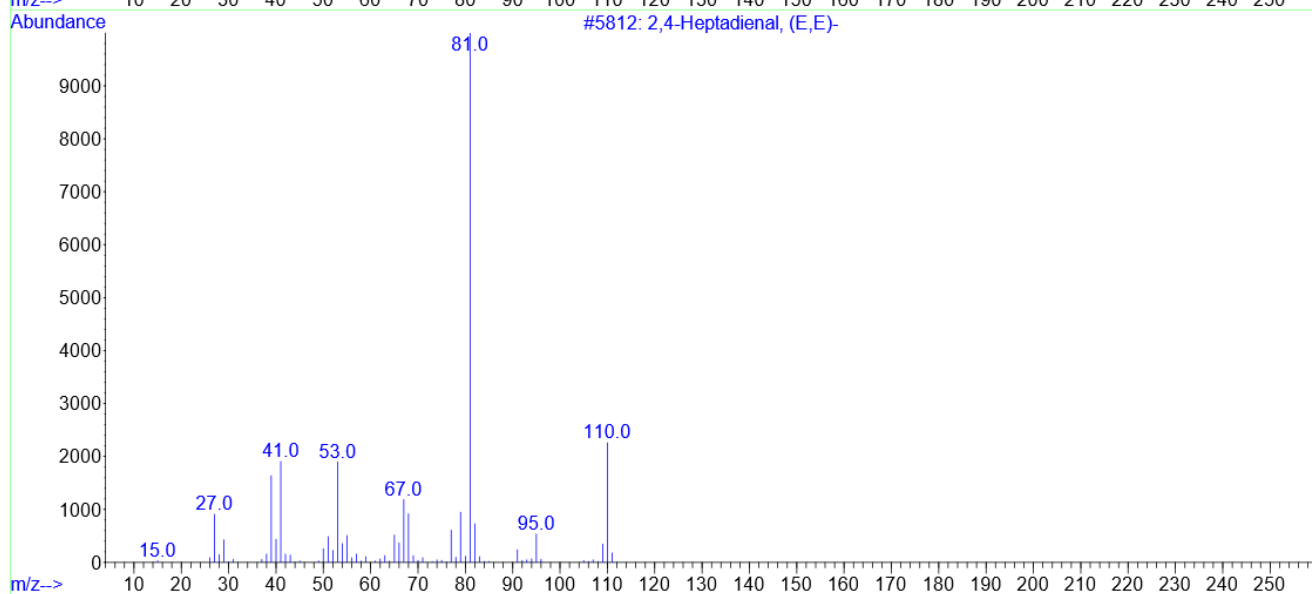
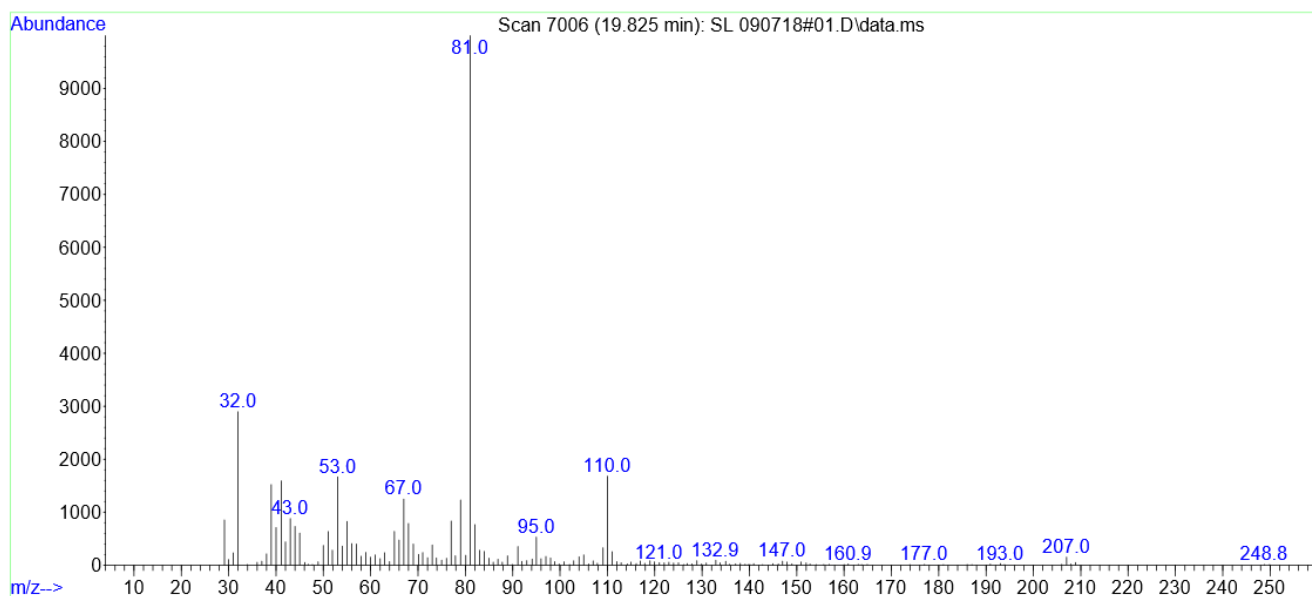
## 51. 2,4-heptadienal isomer 2



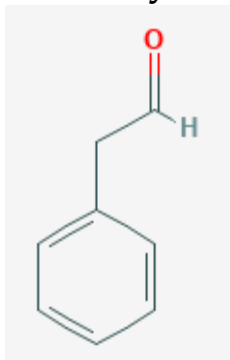
Library Searched : C:\Database\NIST11.L

Quality : 95

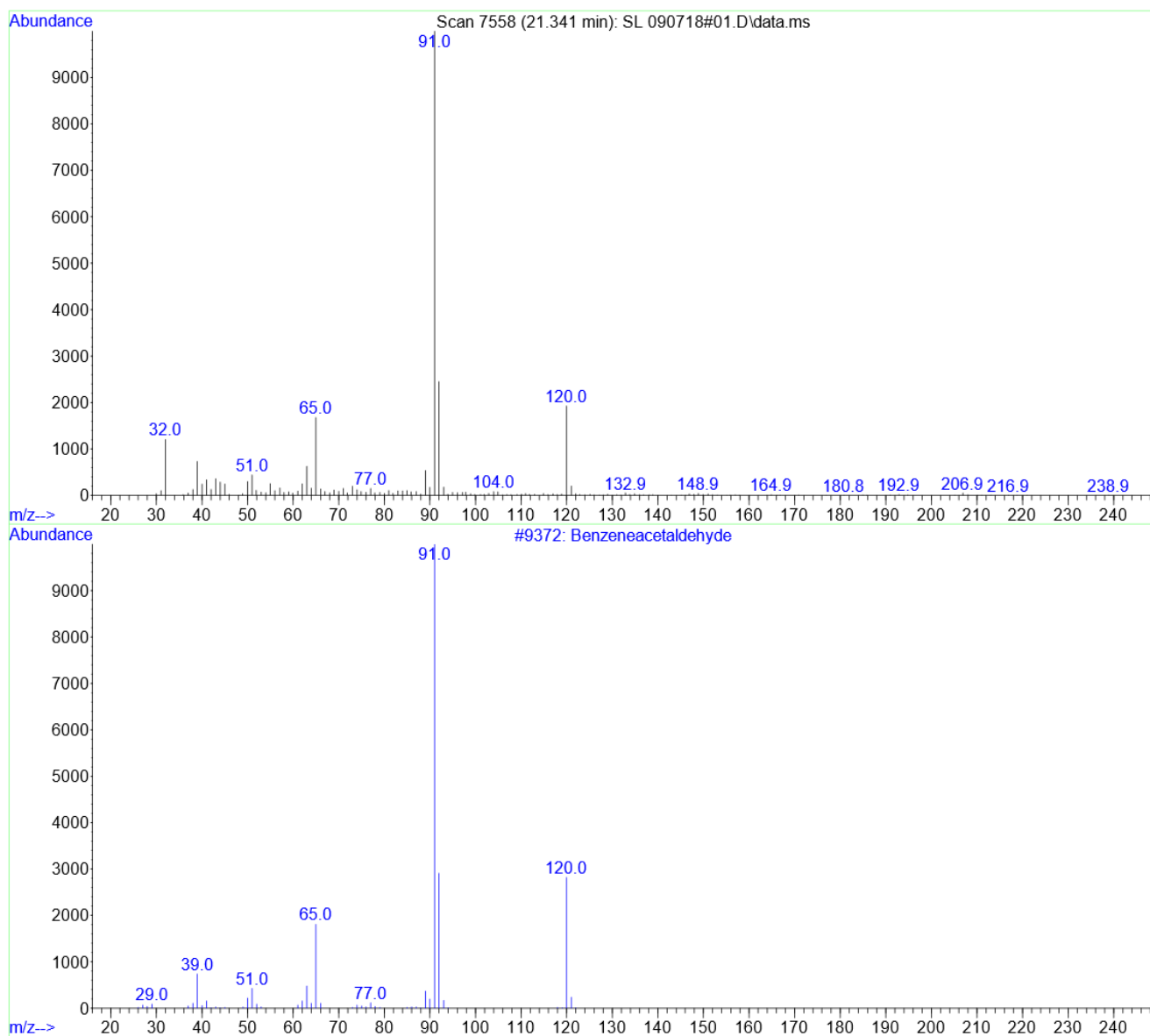
ID : 2,4-Heptadienal, (E,E)-



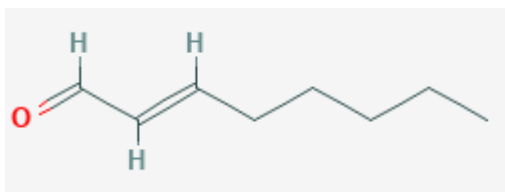
## 52. Phenylacetaldehyde



Library Searched : C:\Database\NIST11.L  
Quality : 94  
ID : Benzeneacetaldehyde



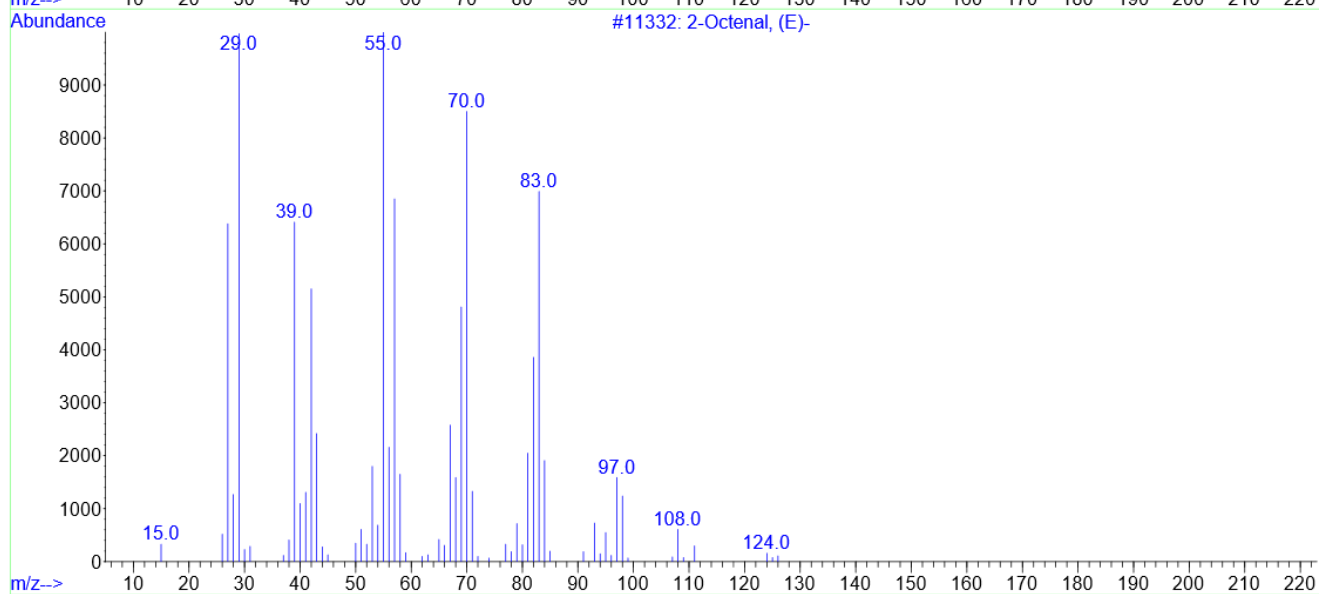
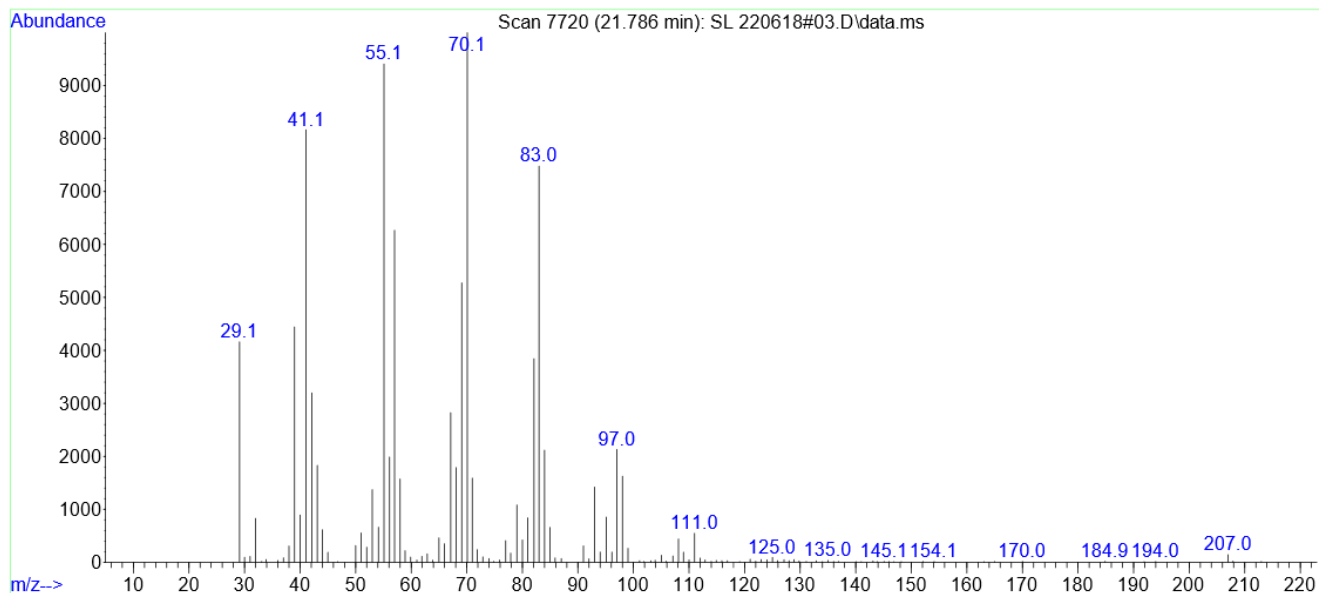
## 53. 2-octenal



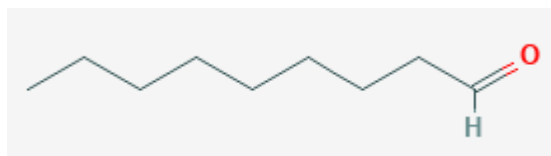
Library Searched : C:\Database\NIST11.L

Quality : 91

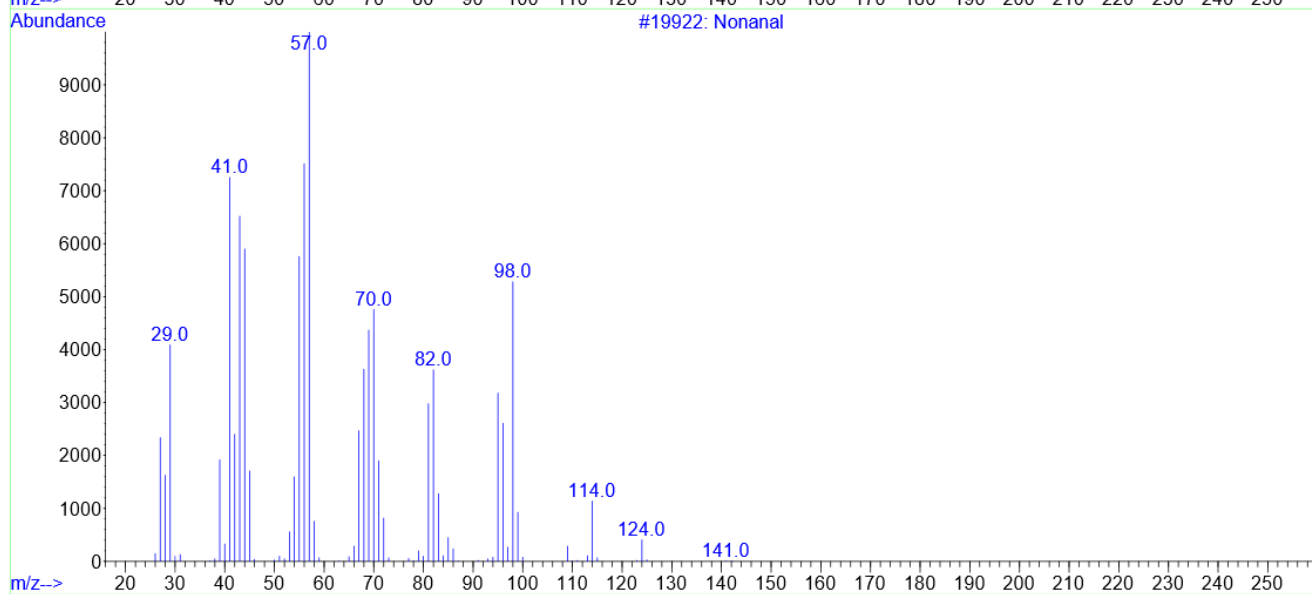
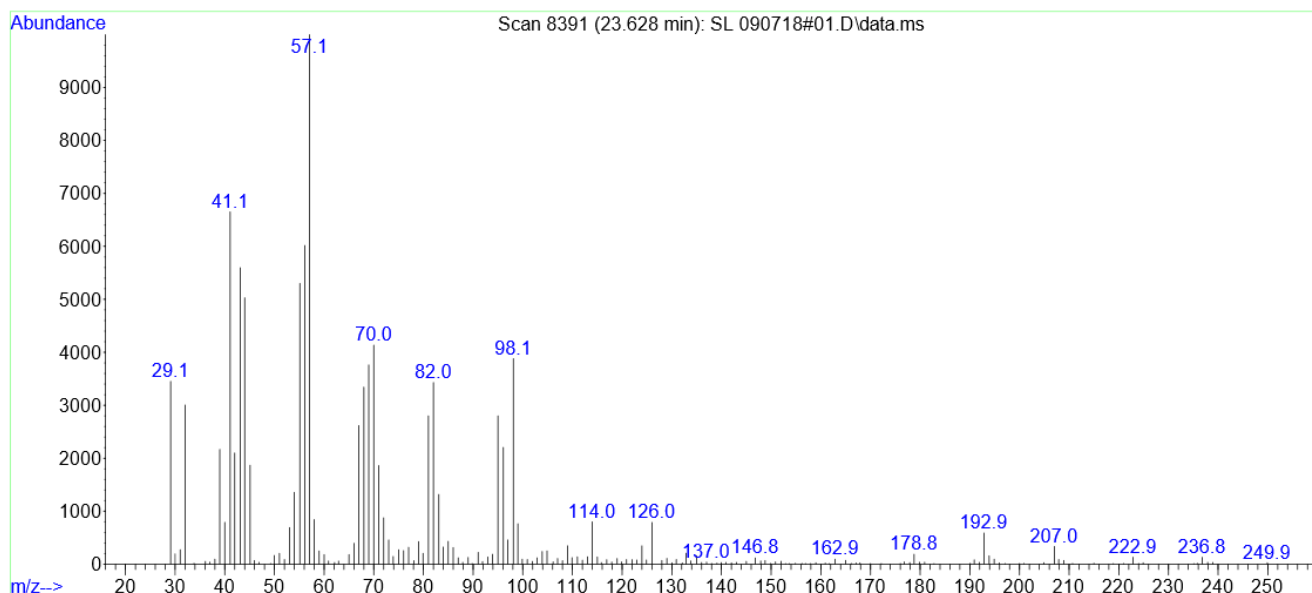
ID : 2-Octenal, (E)-



## 54. Nonanal

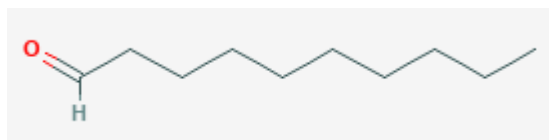


Library Searched : C:\Database\NIST11.L  
Quality : 91  
ID : Nonanal

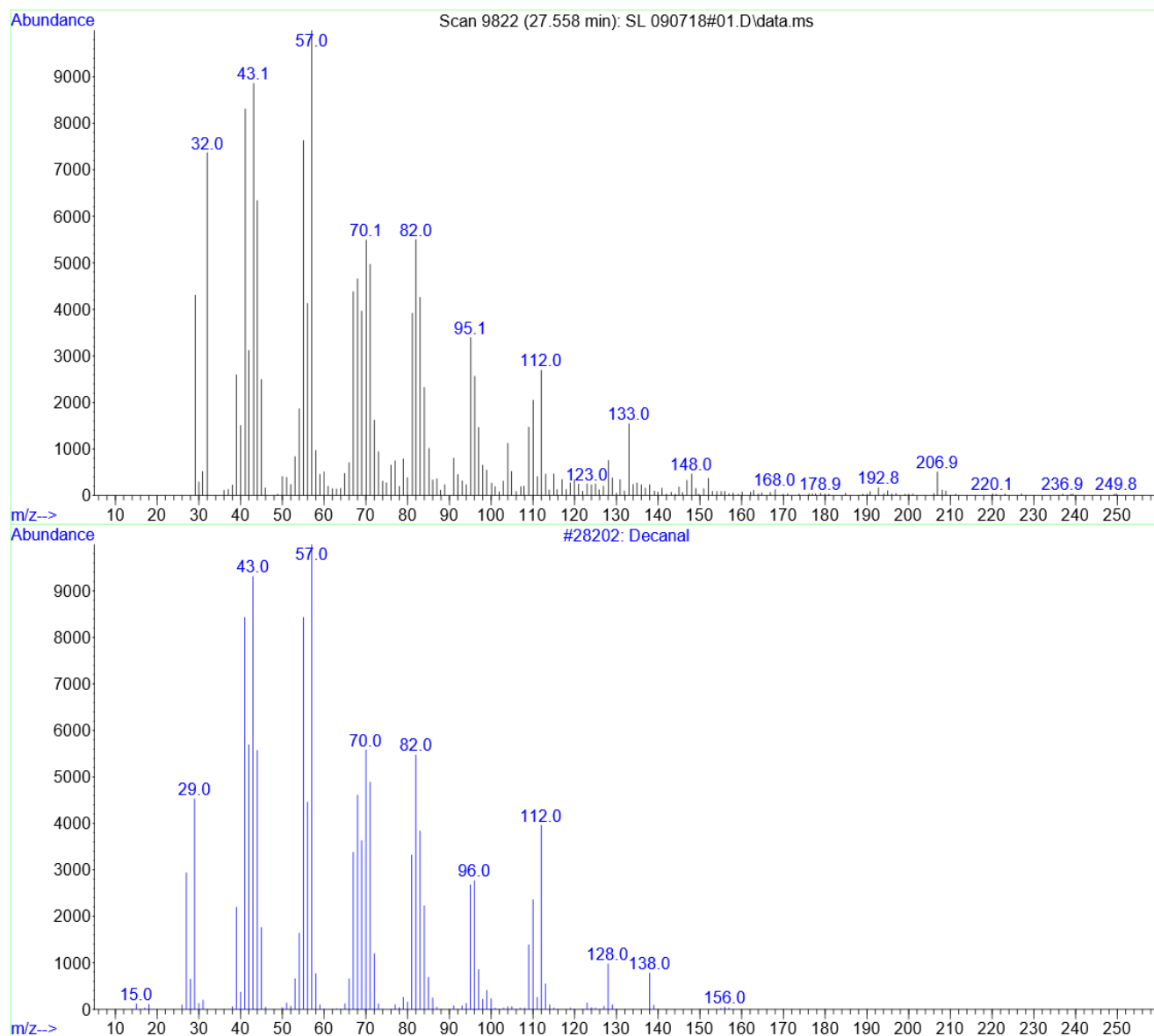




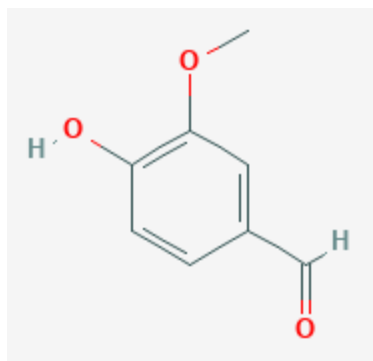
## 55. Decanal



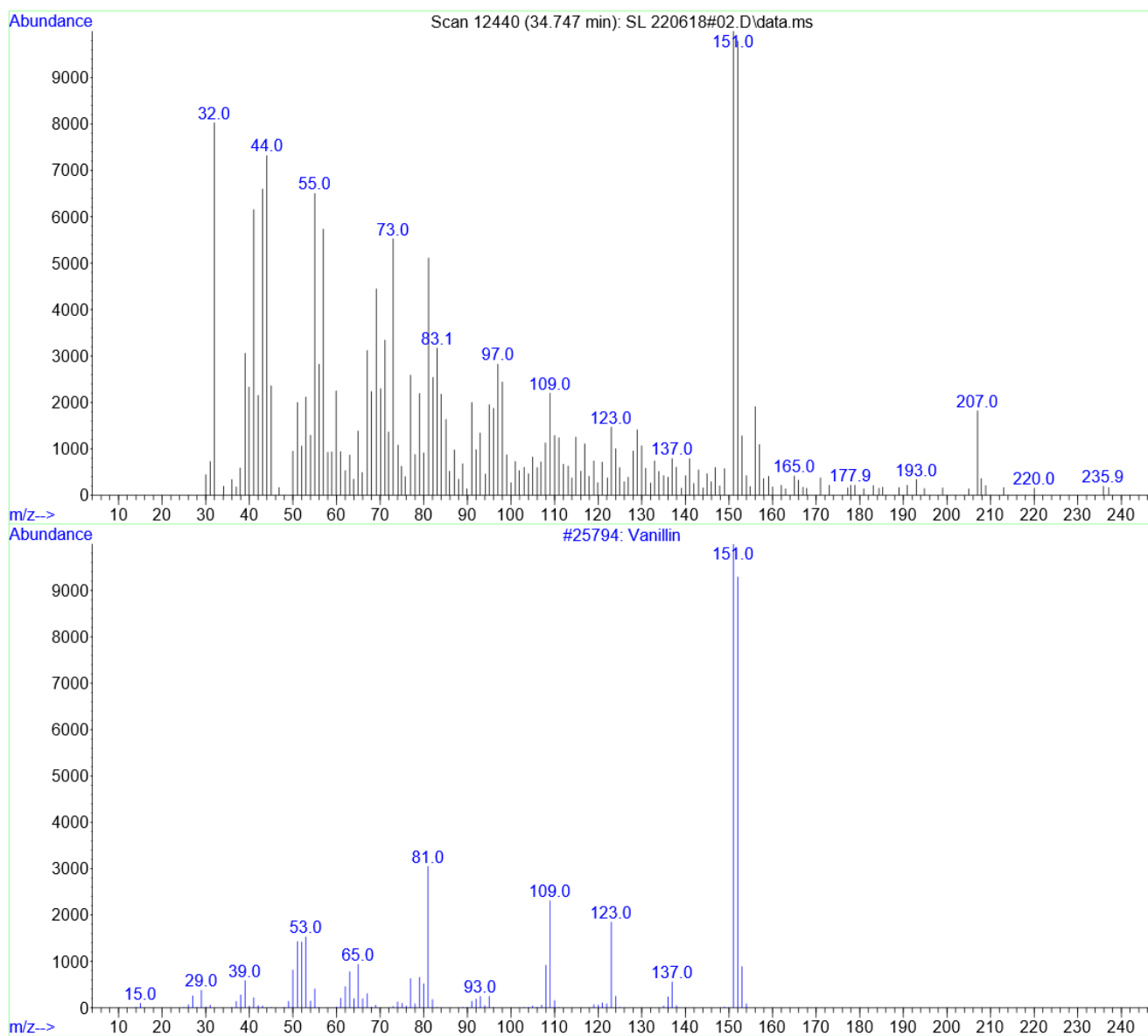
Library Searched : C:\Database\NIST11.L  
Quality : 93  
ID : Decanal



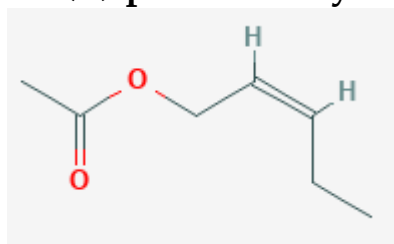
## 56. Vanillin



Library Searched : C:\Database\NIST11.L  
Quality : 83  
ID : Vanillin



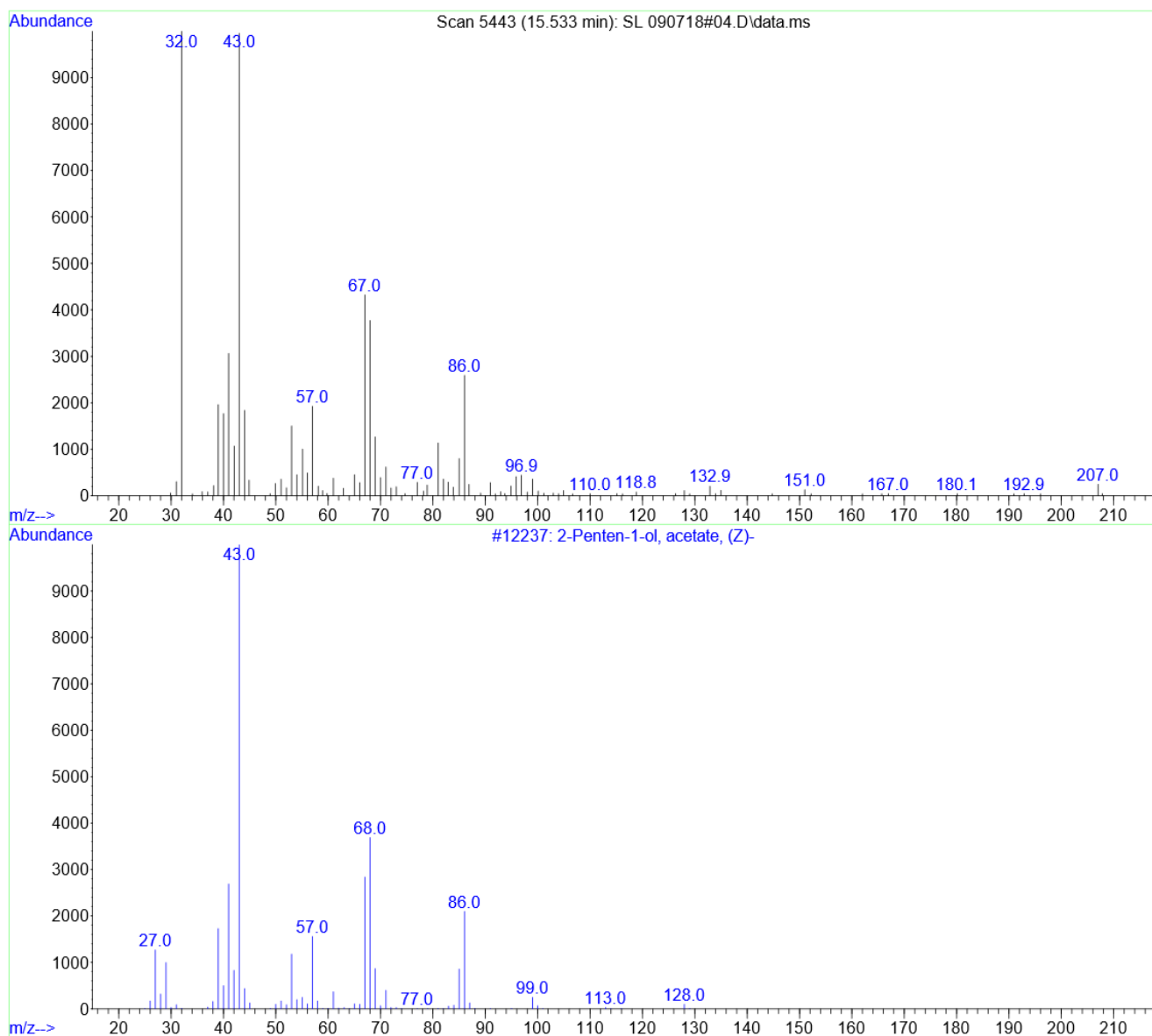
## 57. (Z)-pent-2-en-1-yl acetate



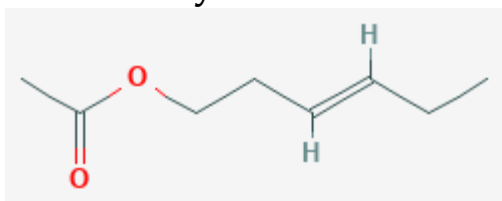
Library Searched : C:\Database\NIST11.L

Quality : 64

ID : 2-Penten-1-ol, acetate, (Z)-



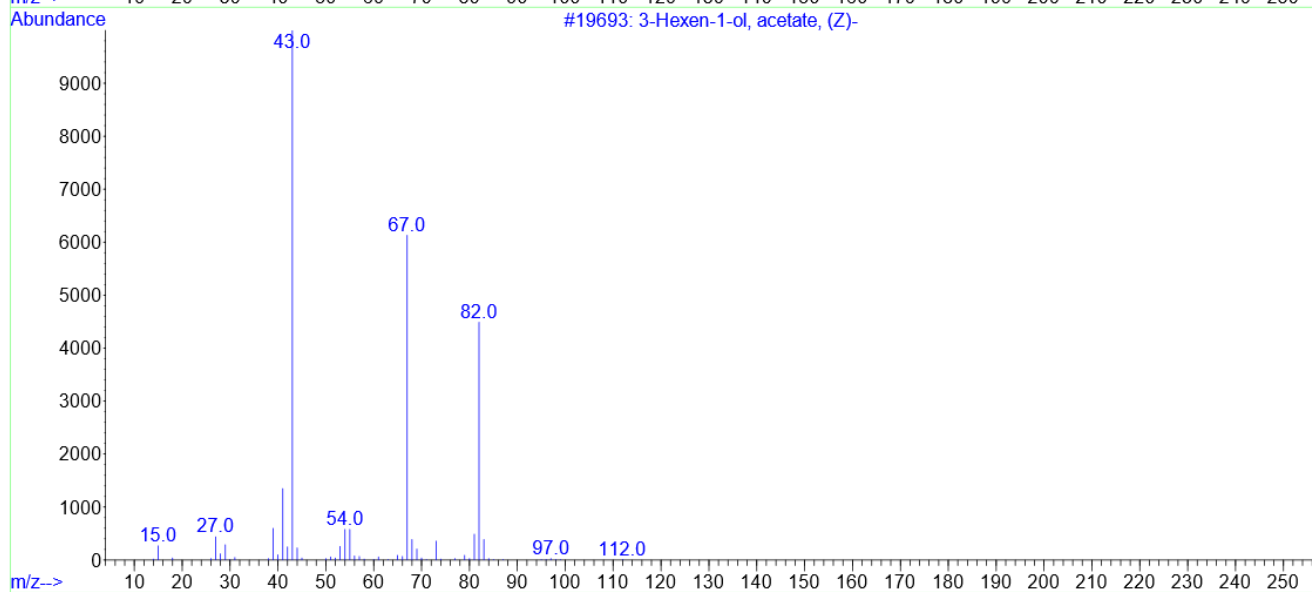
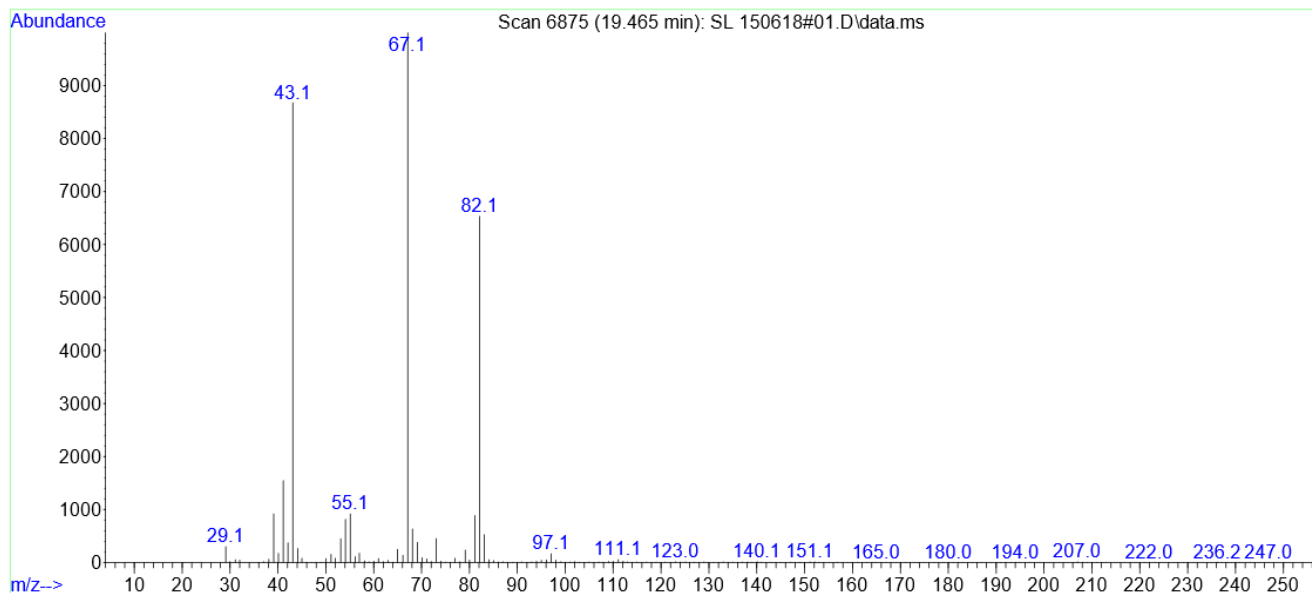
## 58. 3-hexenyl acetate



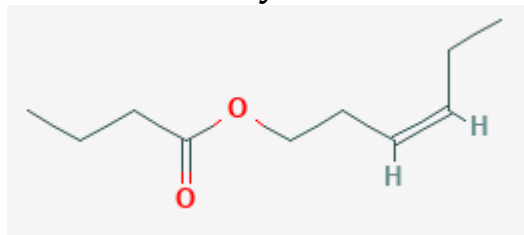
Library Searched : C:\Database\NIST11.L

Quality : 90

ID : 3-Hexen-1-ol, acetate, (Z)-



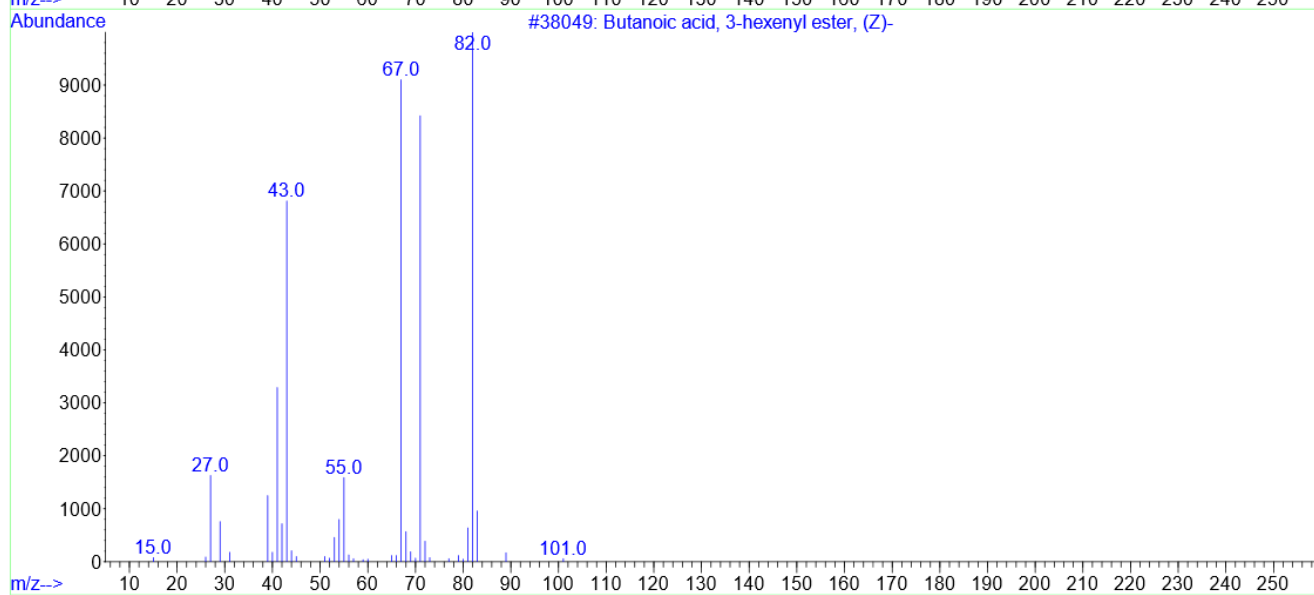
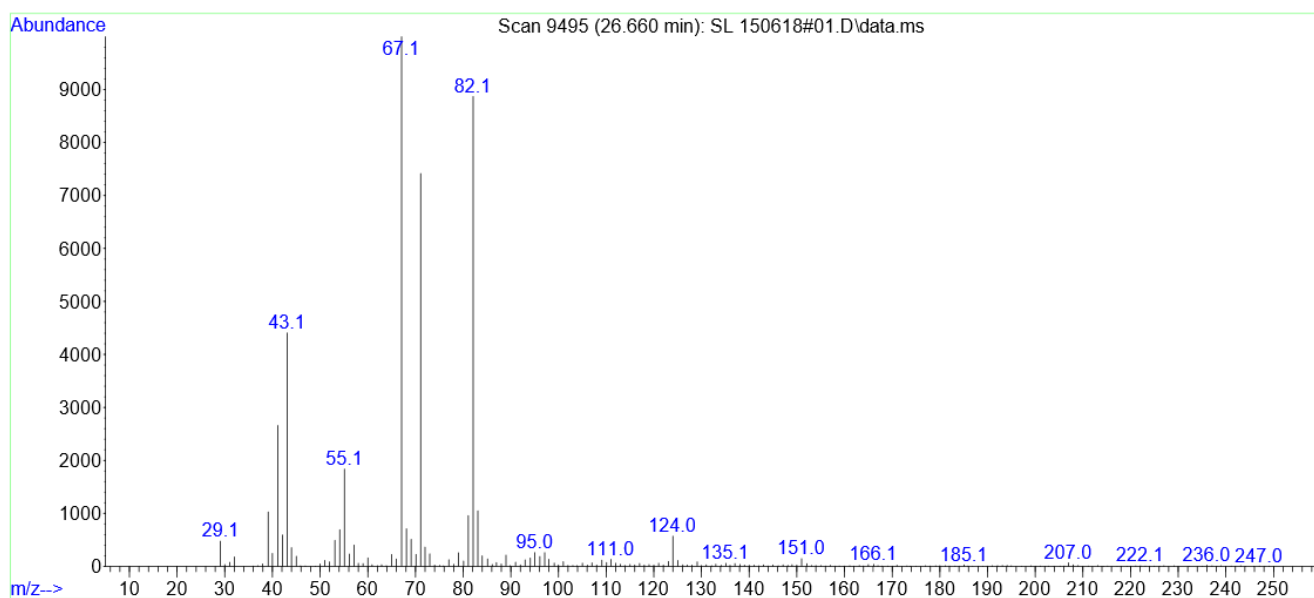
## 59. (Z)-3-hexenyl butanoate



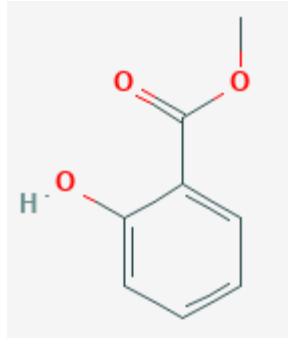
Library Searched : C:\Database\NIST11.L

Quality : 90

ID : Butanoic acid, 3-hexenyl ester, (Z)-



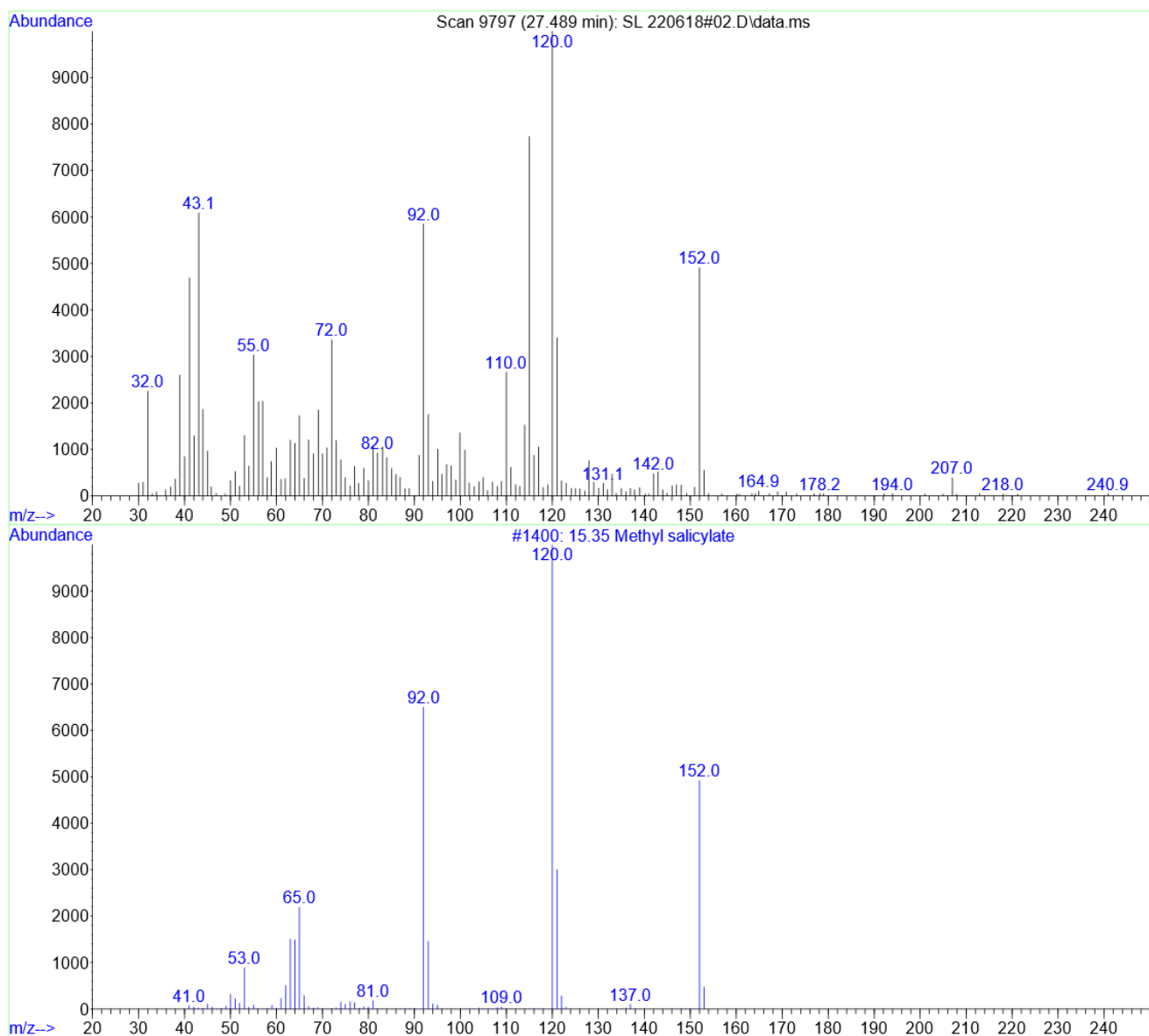
## 60. Methyl salicylate



Library Searched : C:\Database\Adams.L

Quality : 89

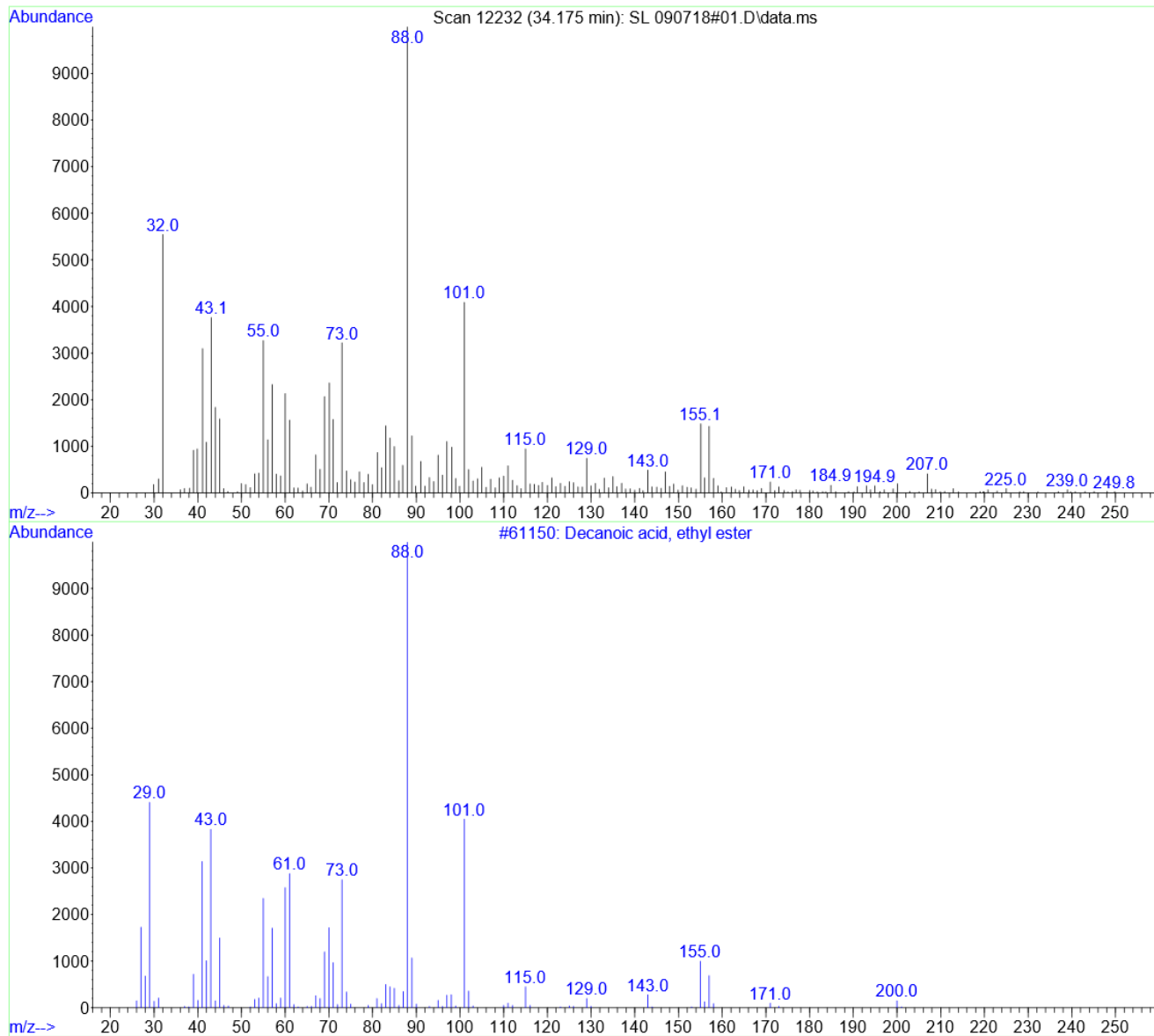
ID : 15.35 Methyl salicylate



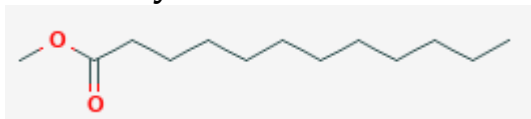
## 61. Ethyl decanoate



Library Searched : C:\Database\NIST11.L  
Quality : 90  
ID : Decanoic acid, ethyl ester



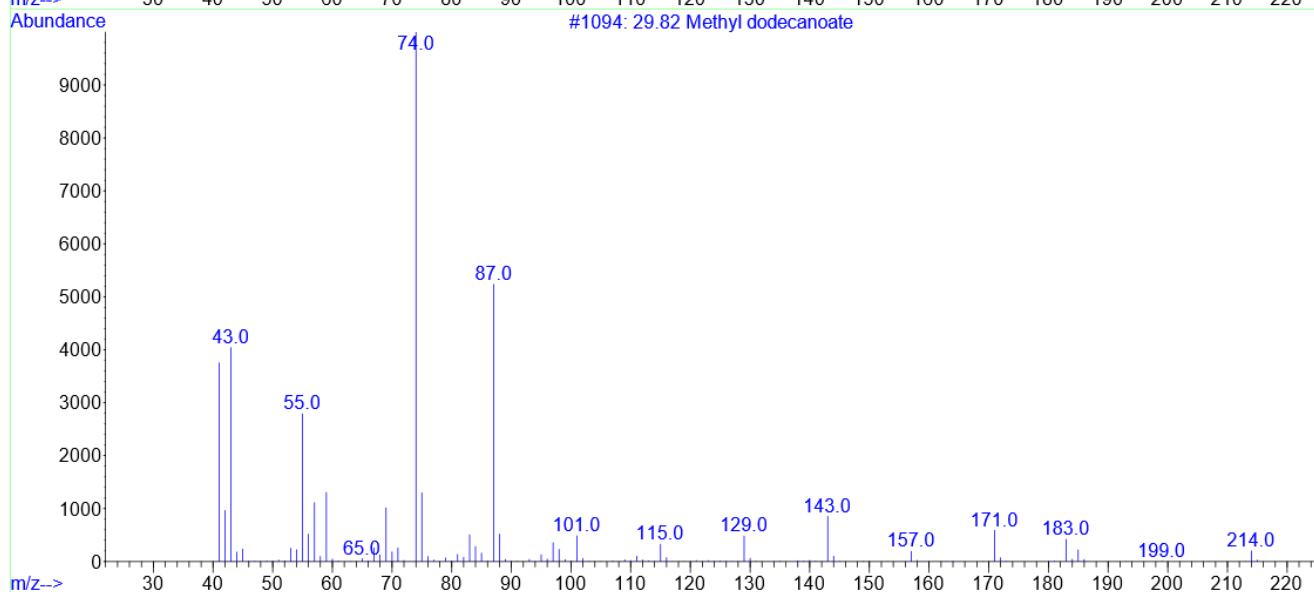
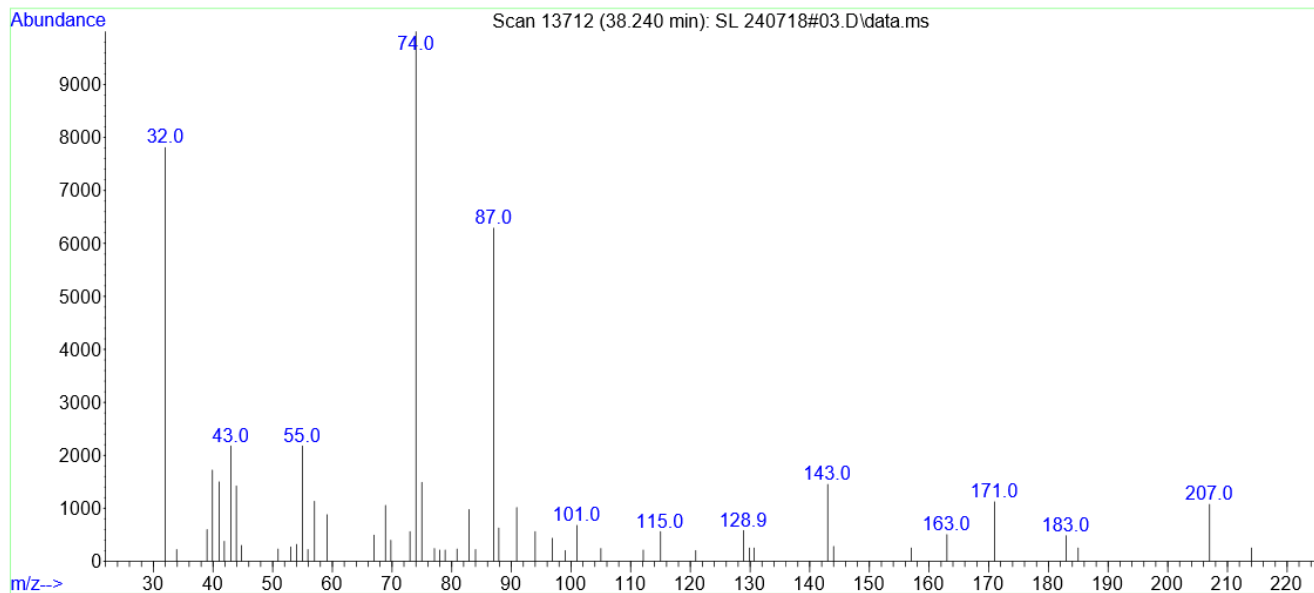
## 62. Methyl dodecanoate



Library Searched : C:\Database\Adams.L

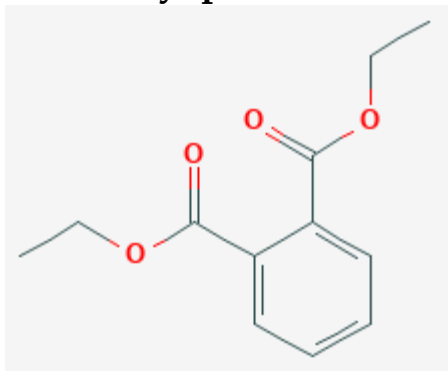
Quality : 93

ID : 29.82 Methyl dodecanoate





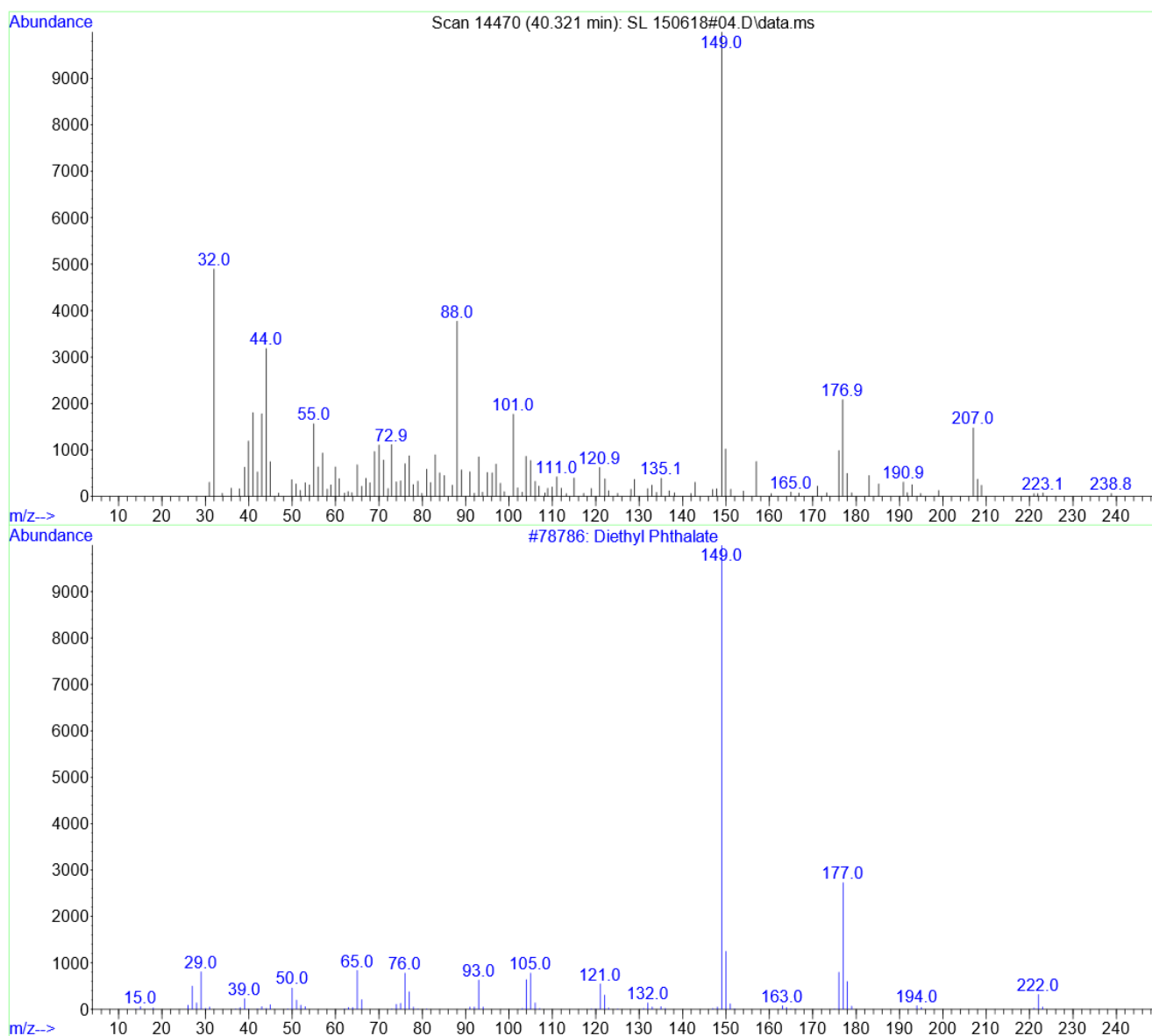
## 63. Diethyl phthalate



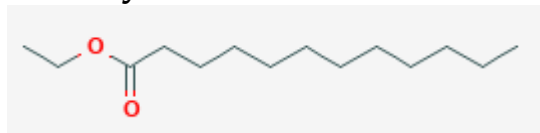
Library Searched : C:\Database\NIST11.L

Quality : 90

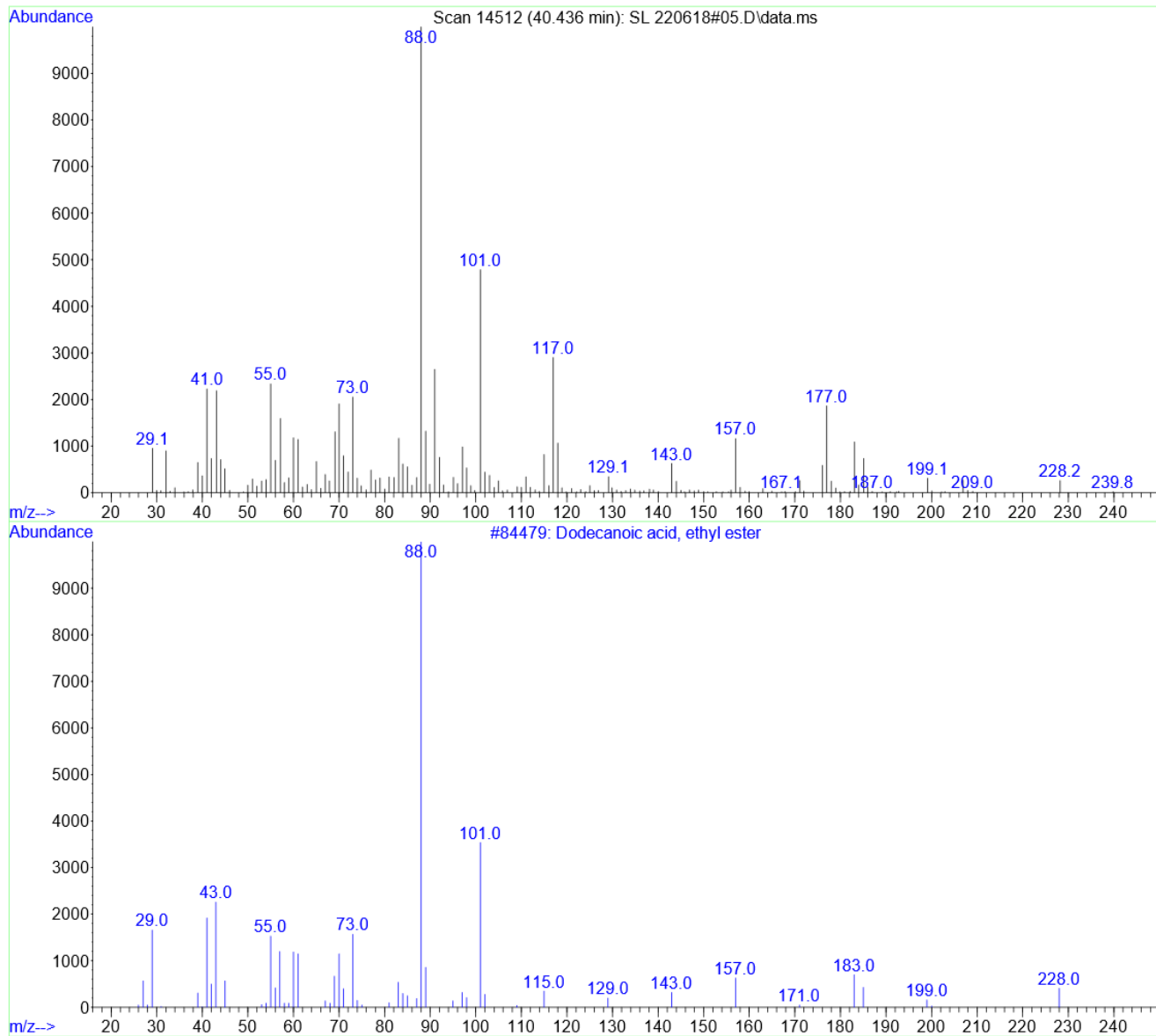
ID : Diethyl Phthalate



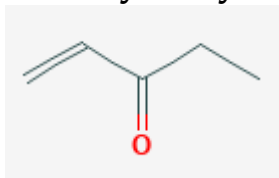
## 64. Ethyl laurate



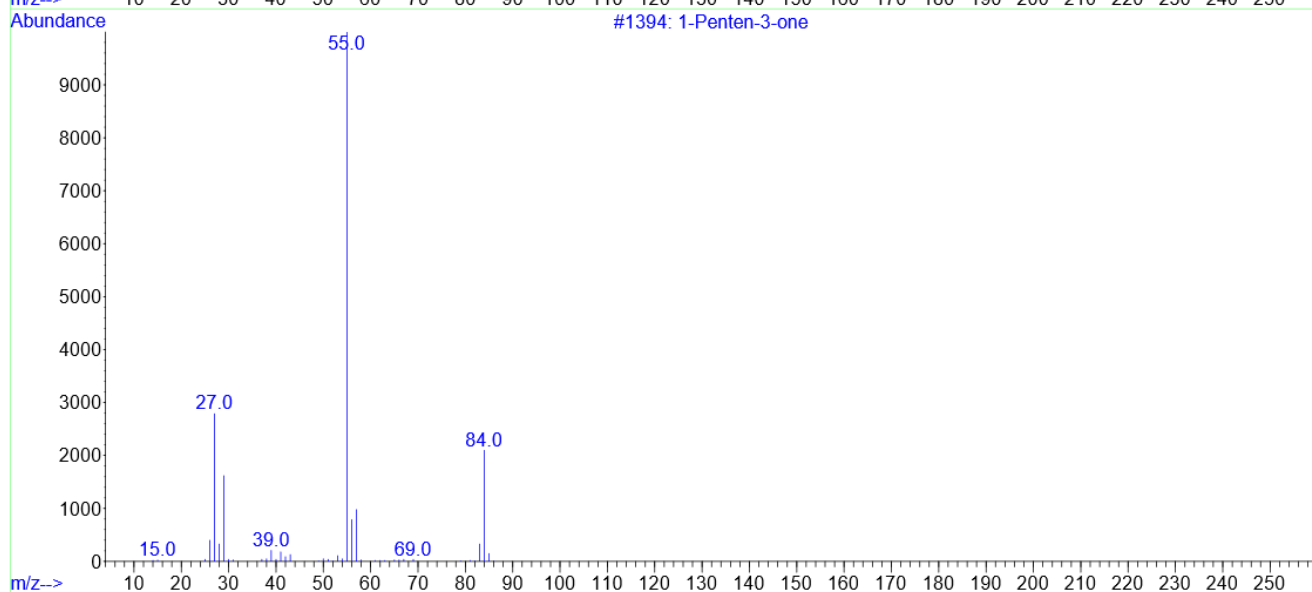
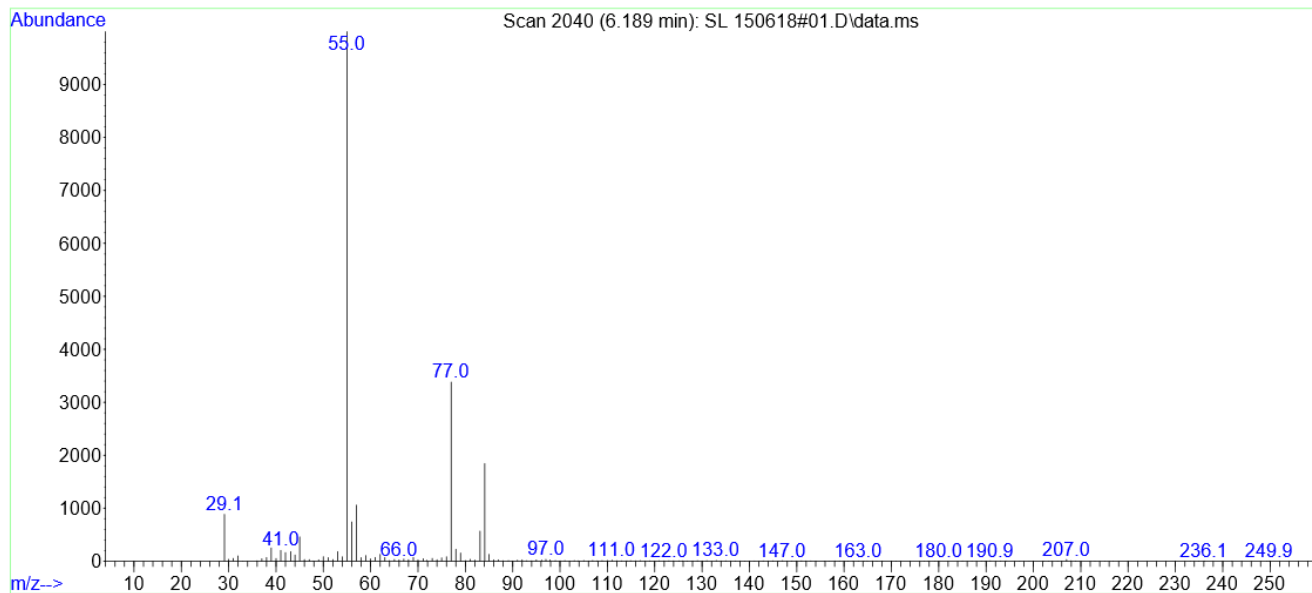
Library Searched : C:\Database\NIST11.L  
Quality : 68  
ID : Dodecanoic acid, ethyl ester



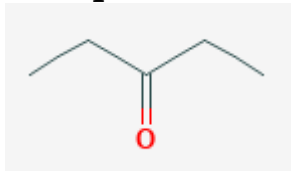
## 65. Ethyl vinyl ketone



Library Searched : C:\Database\NIST11.L  
Quality : 52  
ID : 1-Penten-3-one



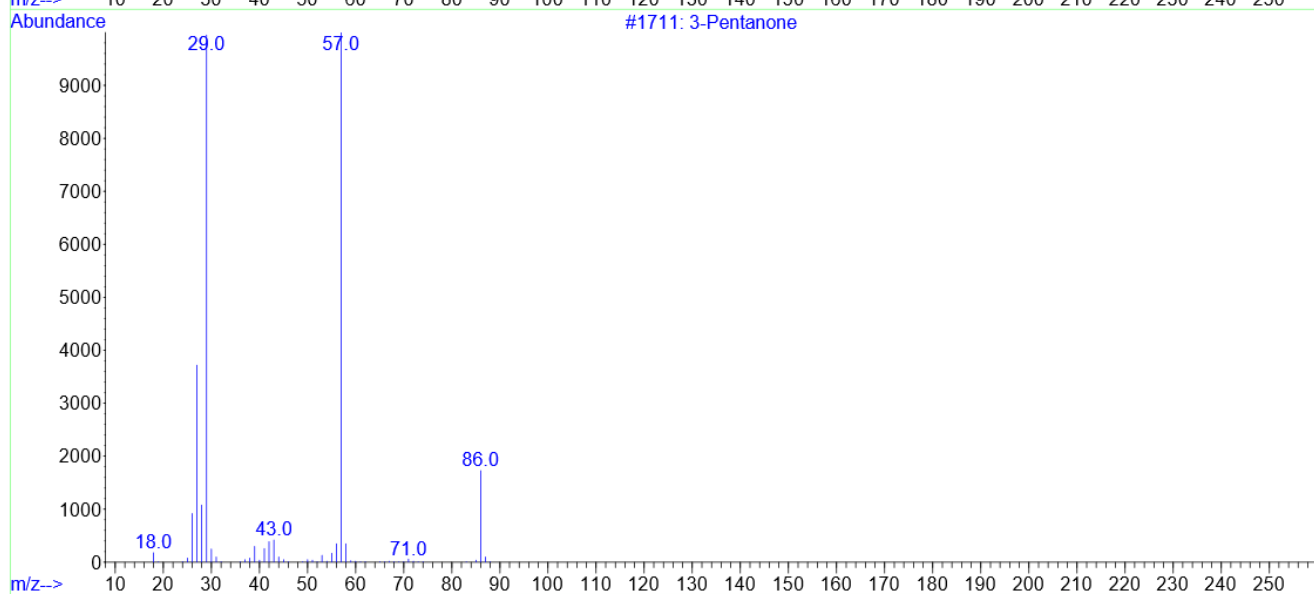
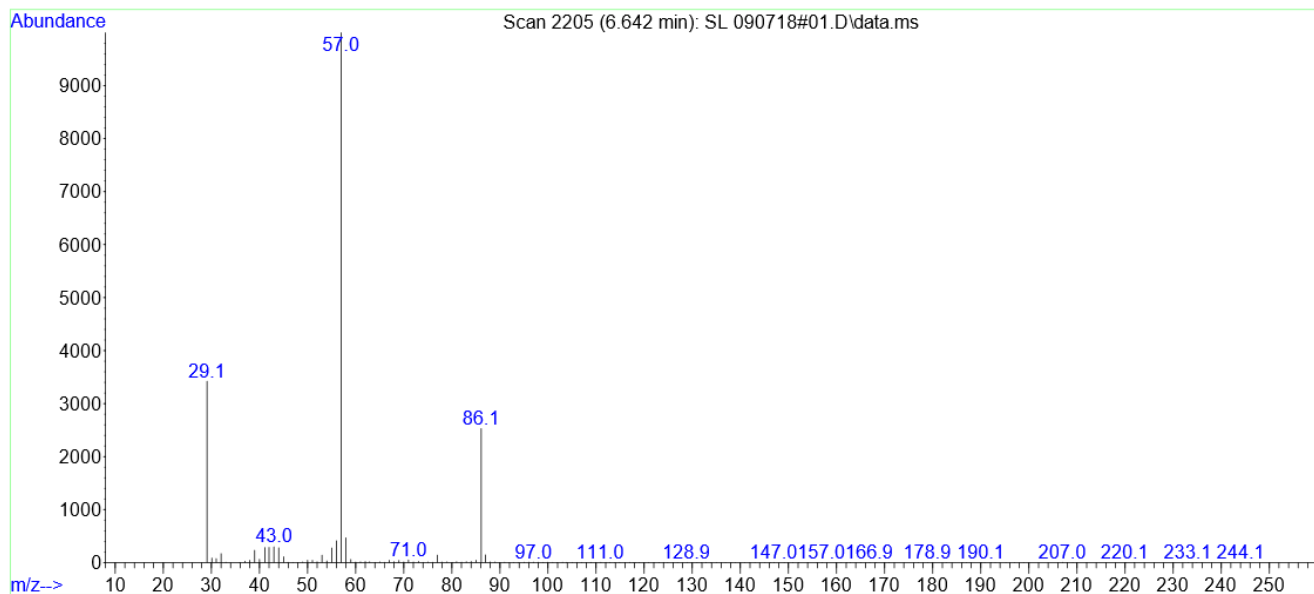
## 66. 3-pentanone



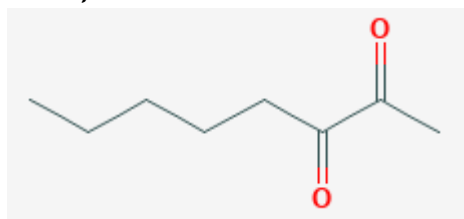
Library Searched : C:\Database\NIST11.L

Quality : 78

ID : 3-Pentanone



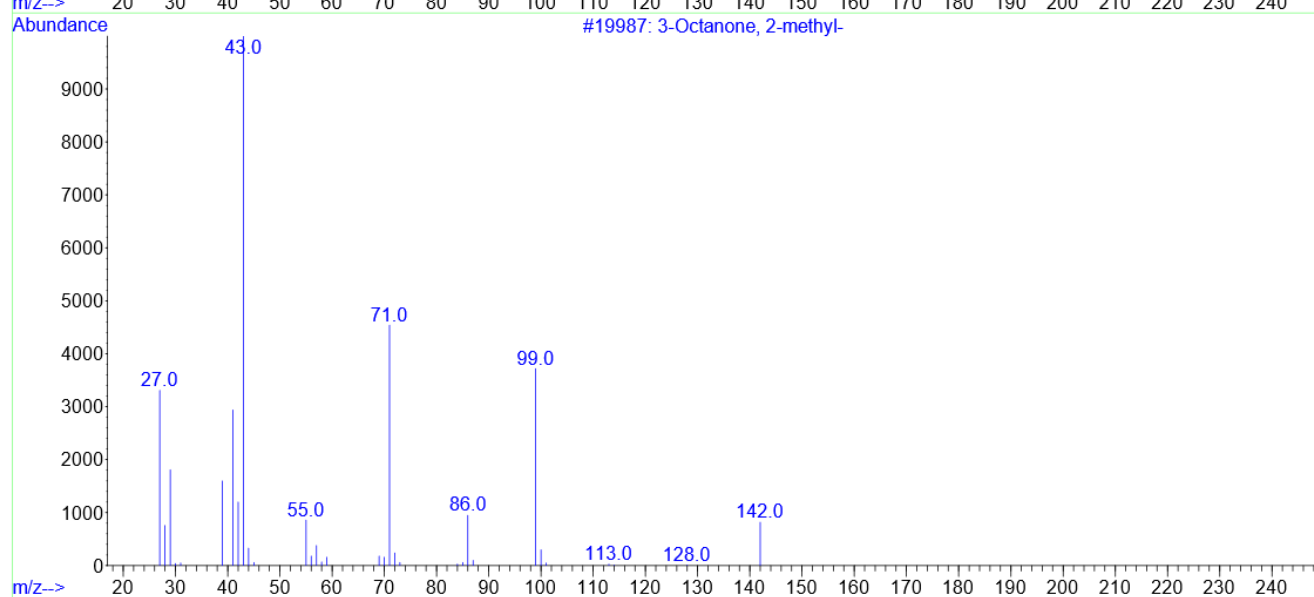
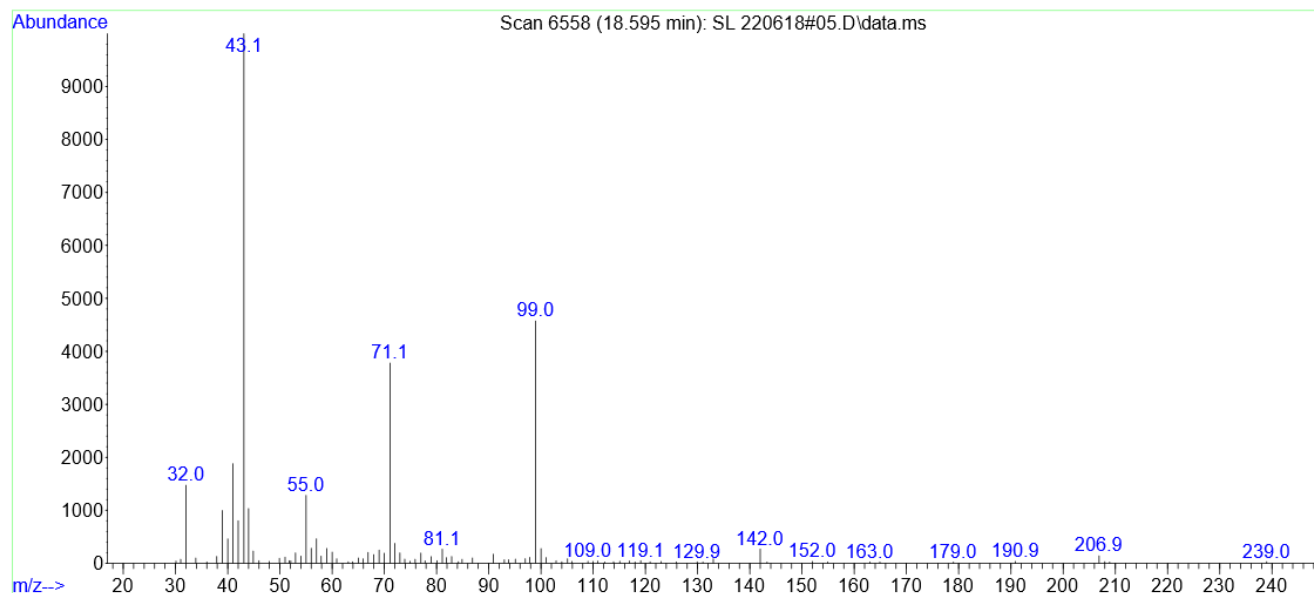
## 67. 2,3-octanedione



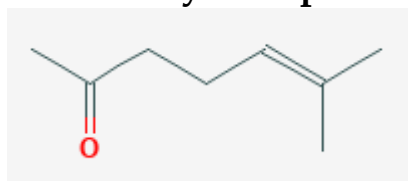
Library Searched : C:\Database\NIST11.L

Quality : 64

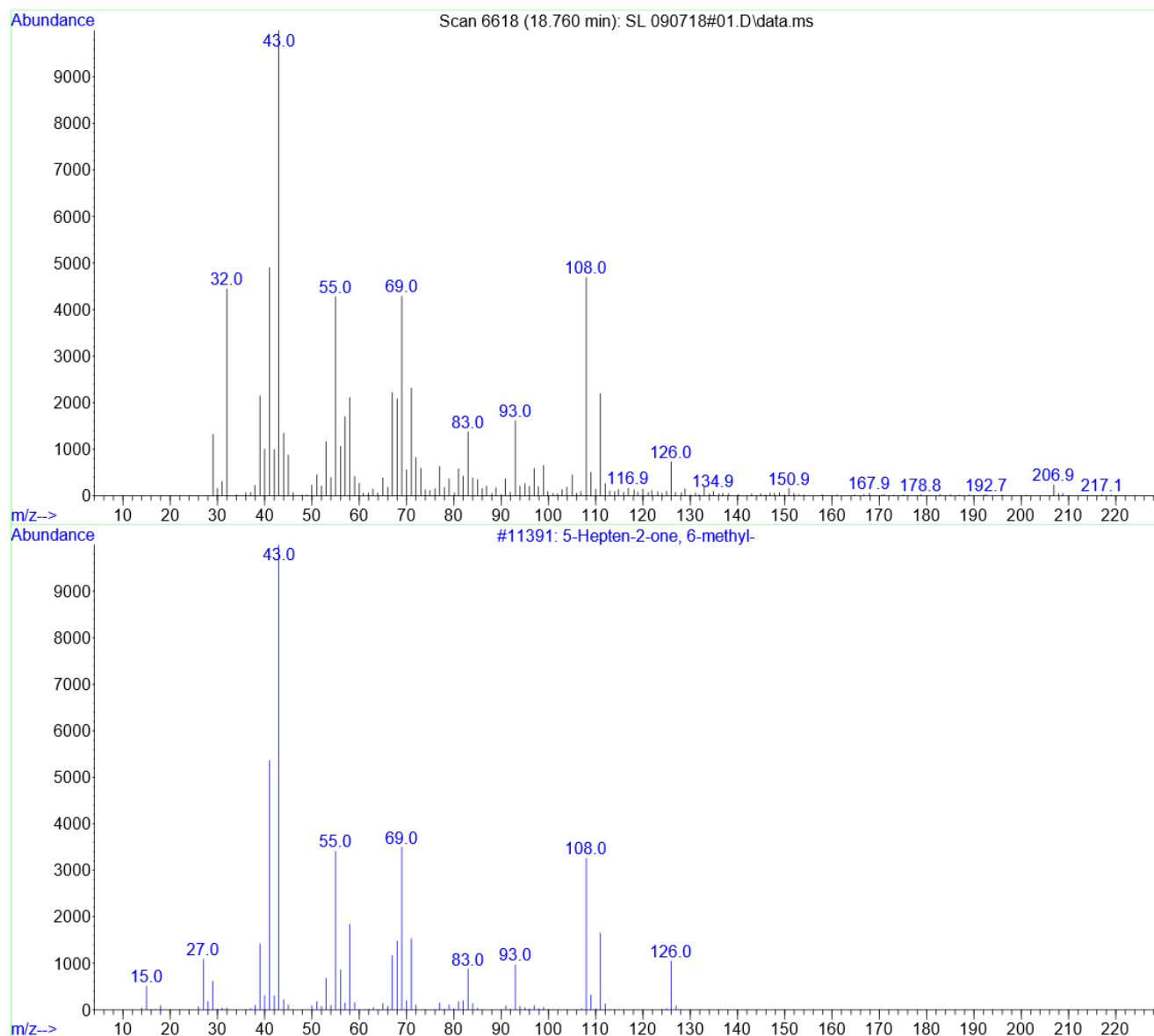
ID : 3-Octanone, 2-methyl-



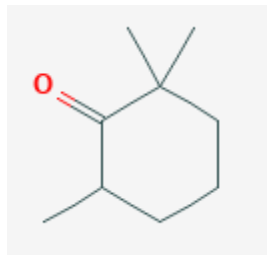
## 68. 6-methyl-5-hepten-2-one



Library Searched : C:\Database\NIST11.L  
Quality : 93  
ID : 5-Hepten-2-one, 6-methyl-



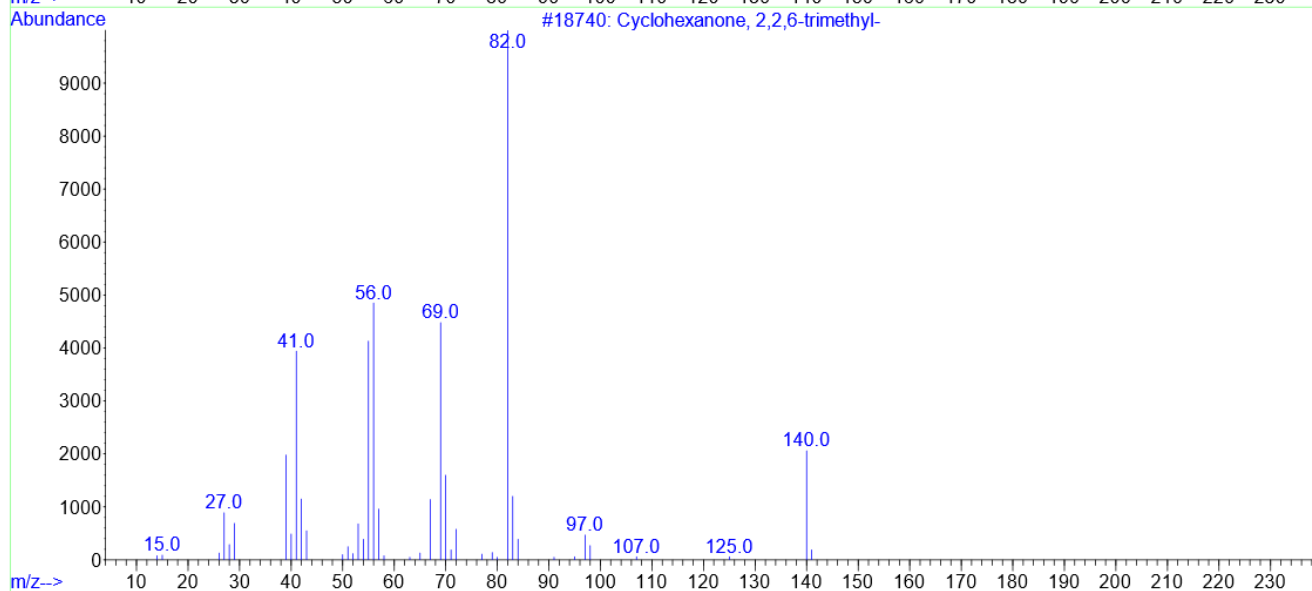
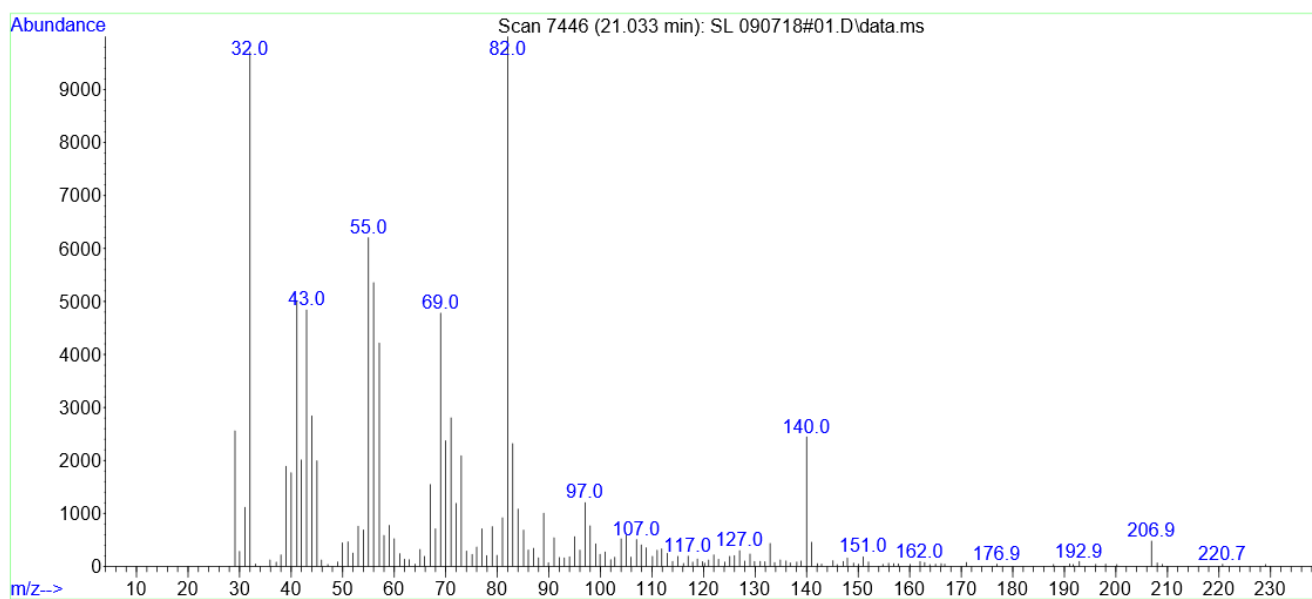
## 69. 2,2,6-trimethylcyclohexanone



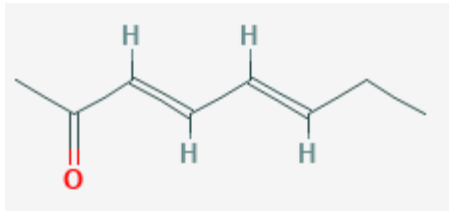
Library Searched : C:\Database\NIST11.L

Quality : 58

ID : Cyclohexanone, 2,2,6-trimethyl-



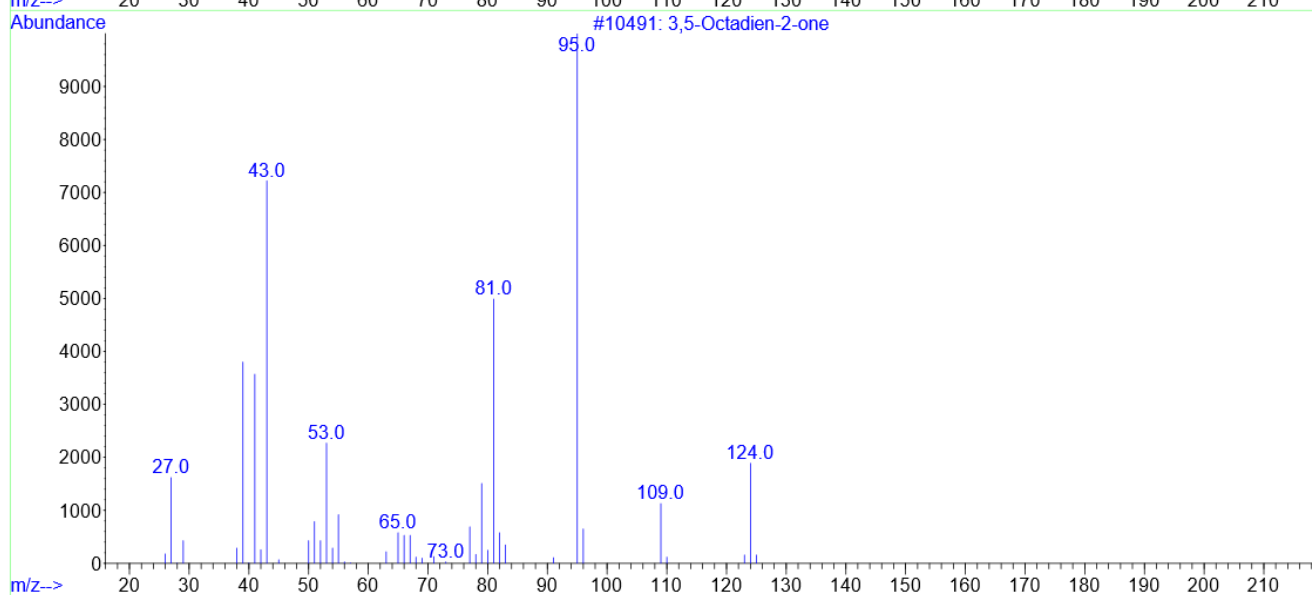
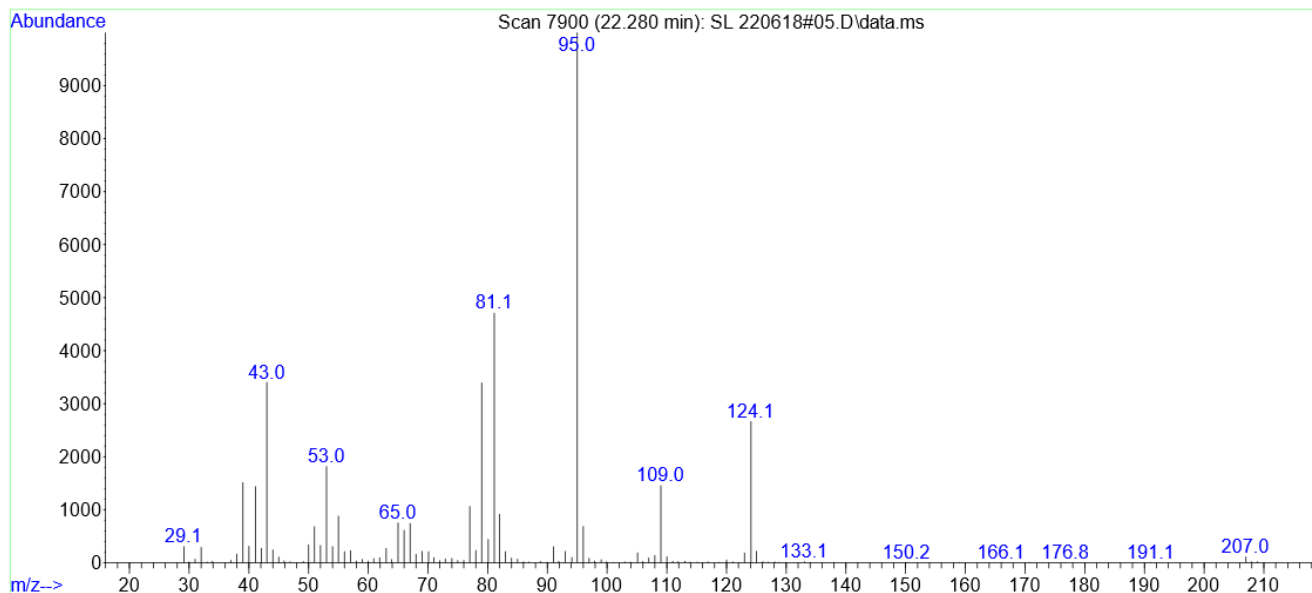
## 70. (E,E)-3,5-octadien-2-one



Library Searched : C:\Database\NIST11.L

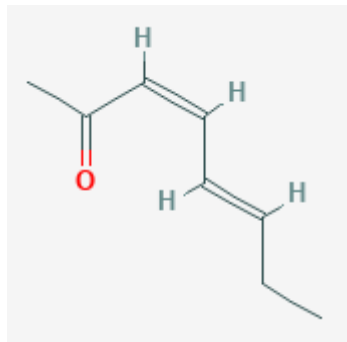
Quality : 87

ID : 3,5-Octadien-2-one





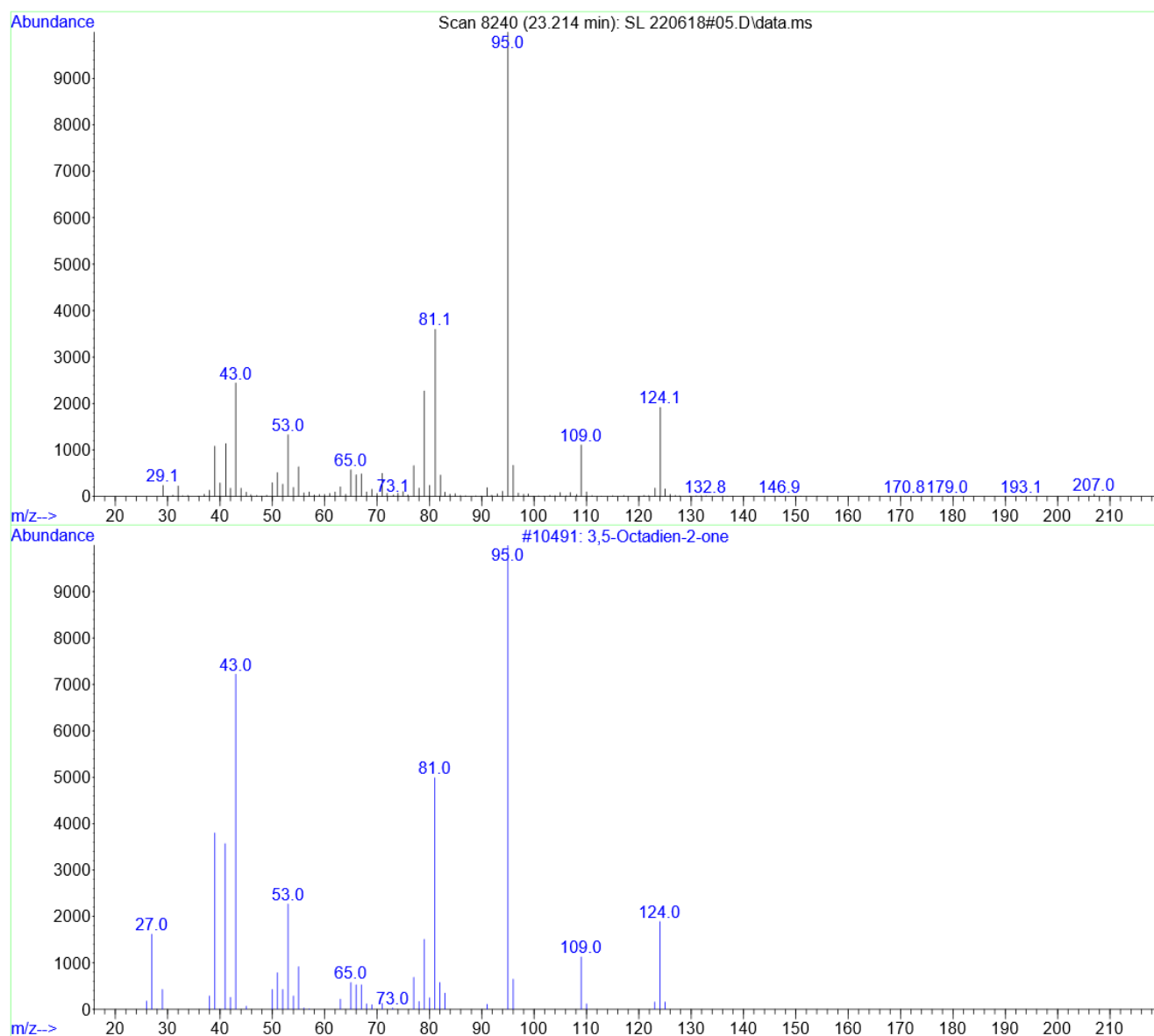
## 71. 3,5-octadien-2-one



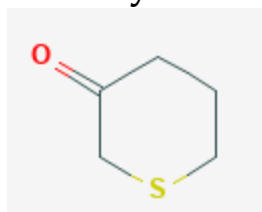
Library Searched : C:\Database\NIST11.L

Quality : 90

ID : 3,5-Octadien-2-one



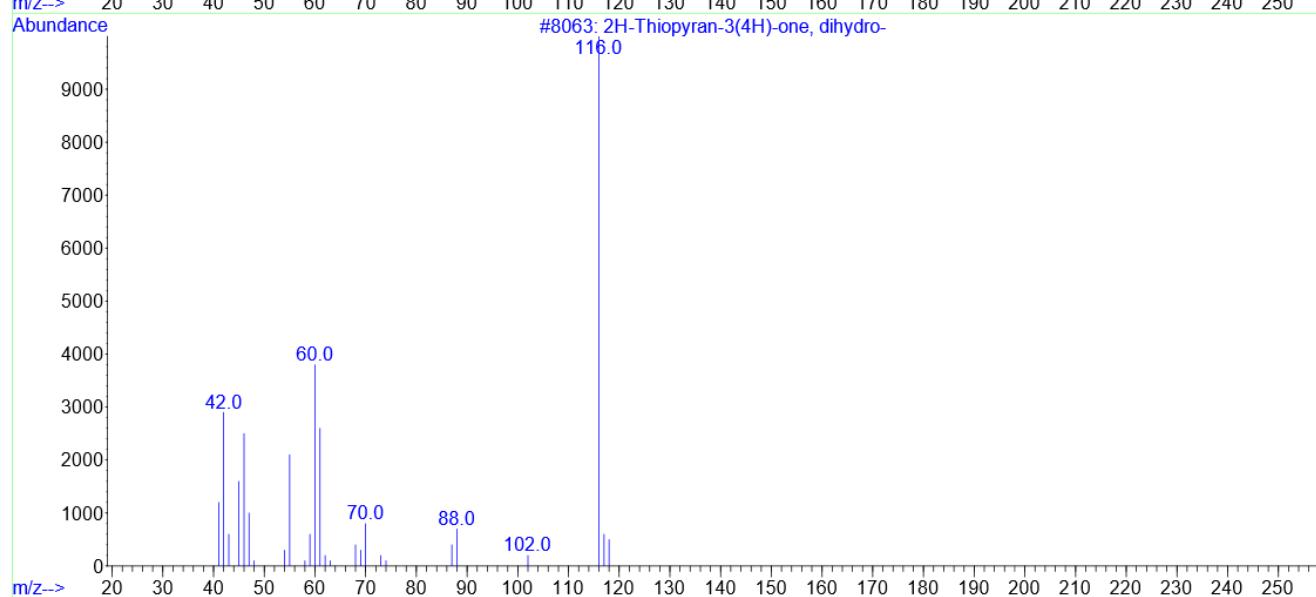
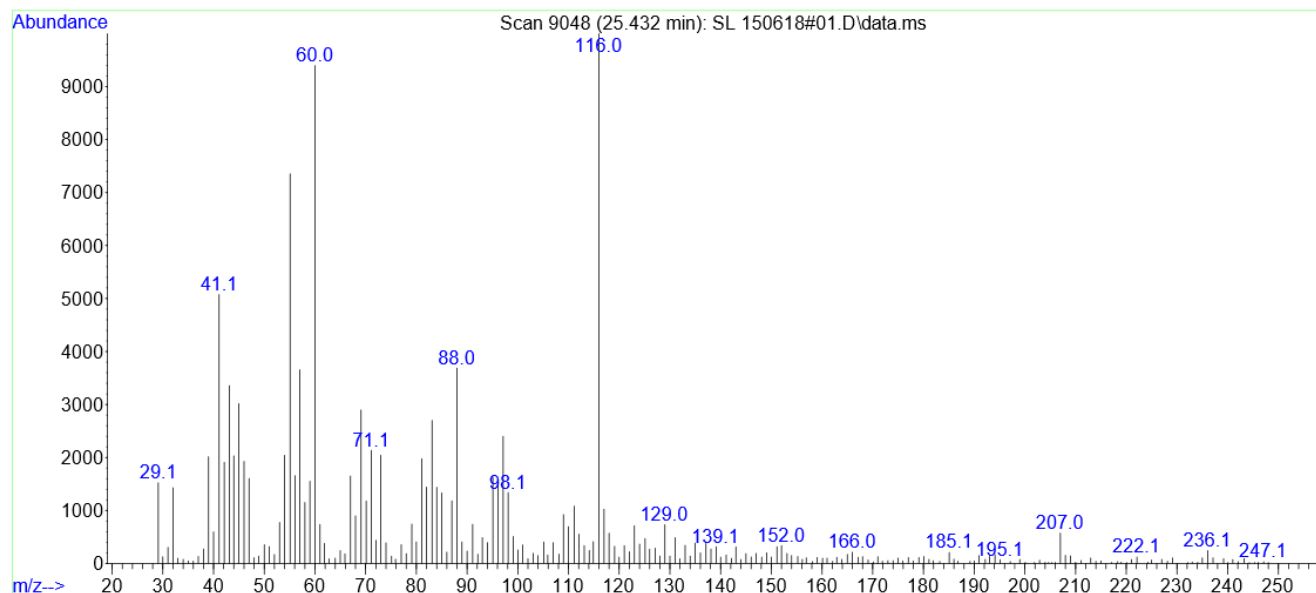
## 72. Dihydro-2H-thiopyran-3(4H)-one



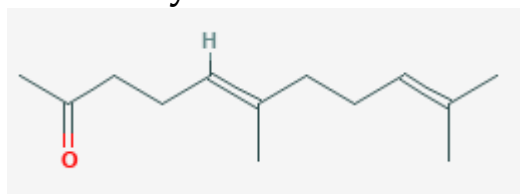
Library Searched : C:\Database\NIST11.L

Quality : 53

ID : 2H-Thiopyran-3(4H)-one, dihydro-



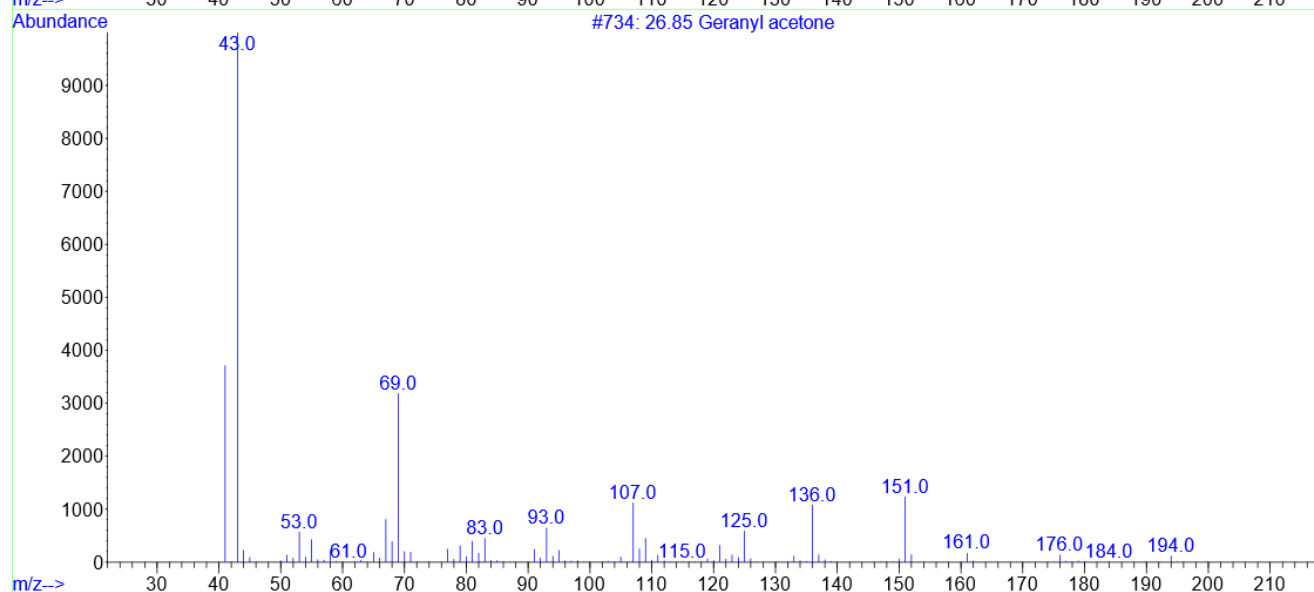
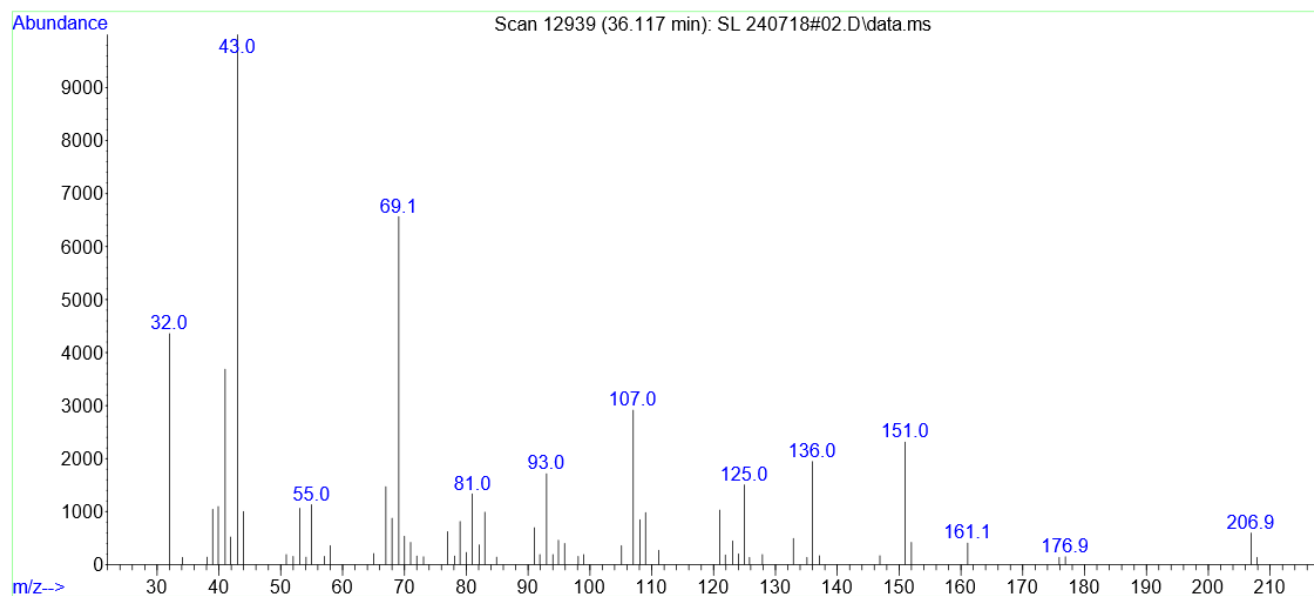
## 73. Geranylacetone



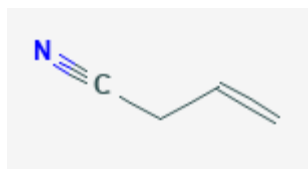
Library Searched : C:\Database\Adams.L

Quality : 78

ID : 26.85 Geranyl acetone



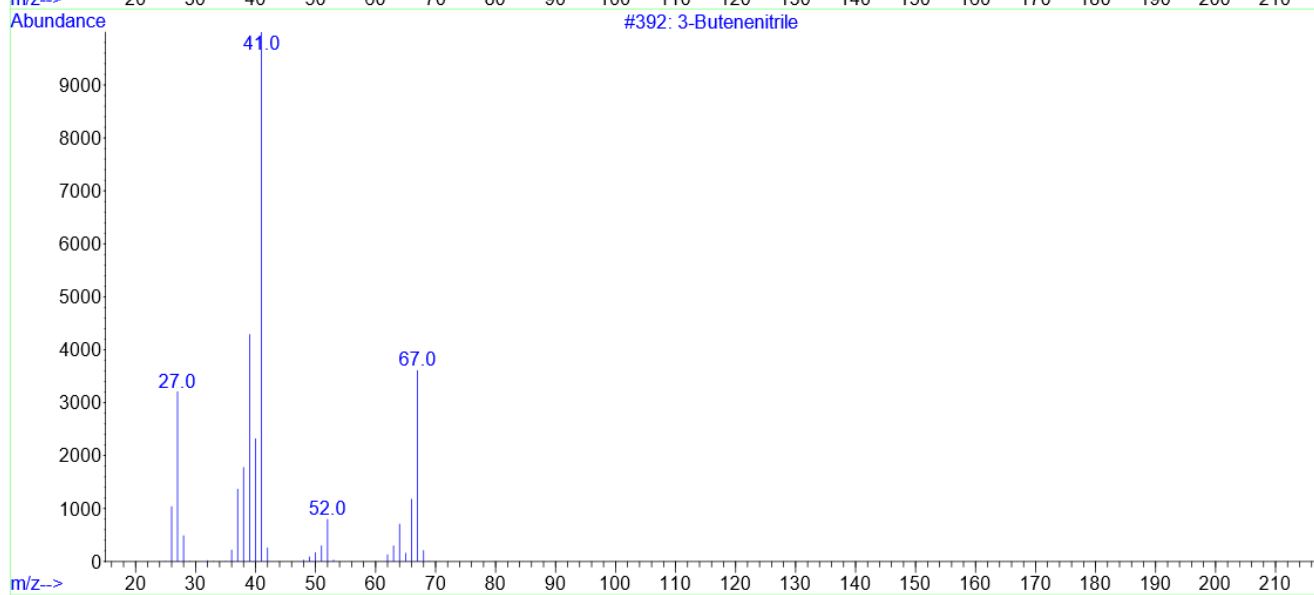
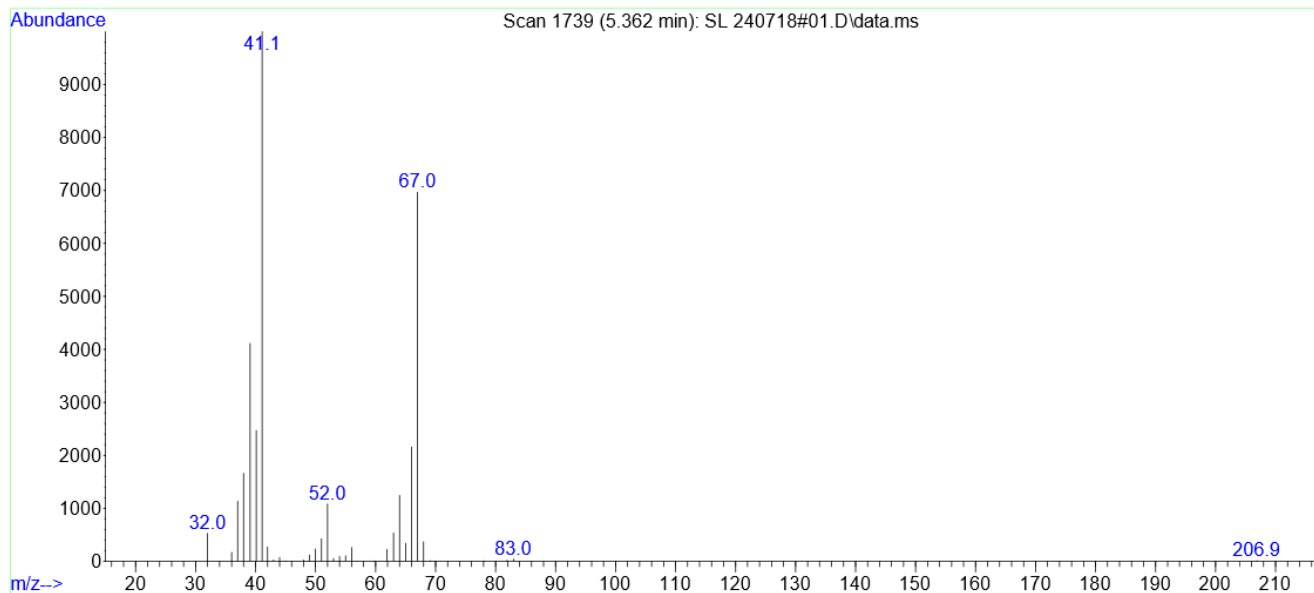
## 74. 3-butenenitrile



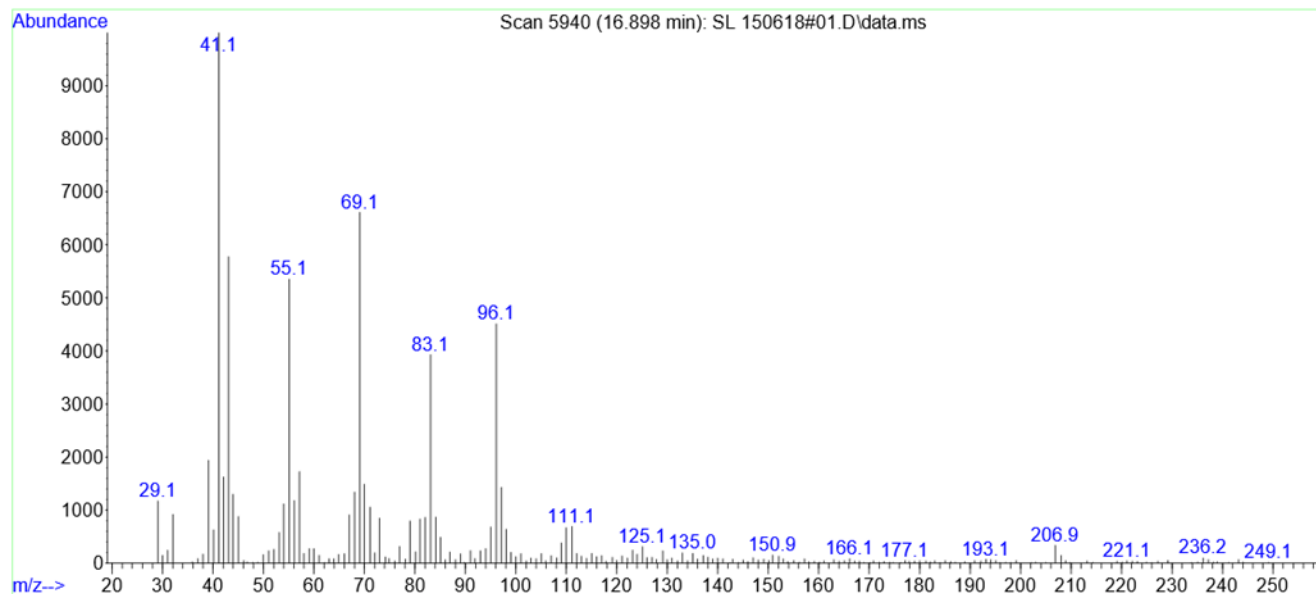
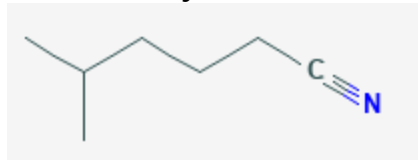
Library Searched : C:\Database\NIST11.L

Quality : 94

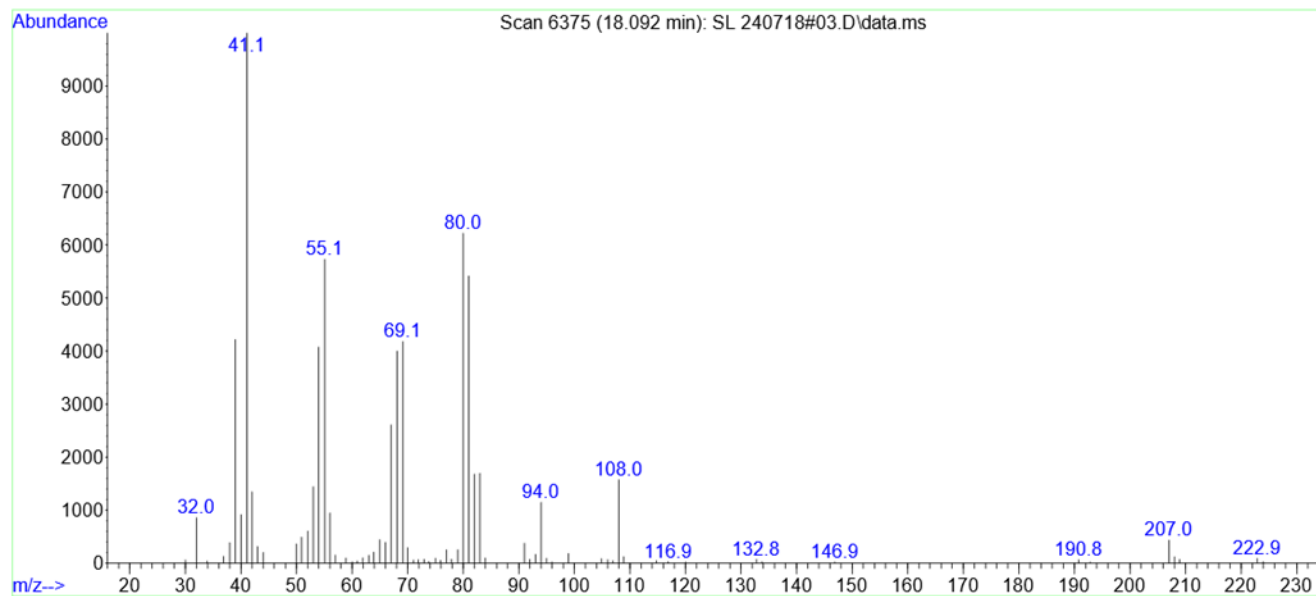
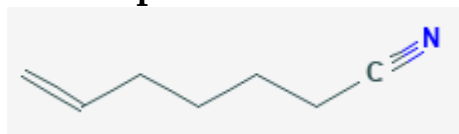
ID : 3-Butenenitrile



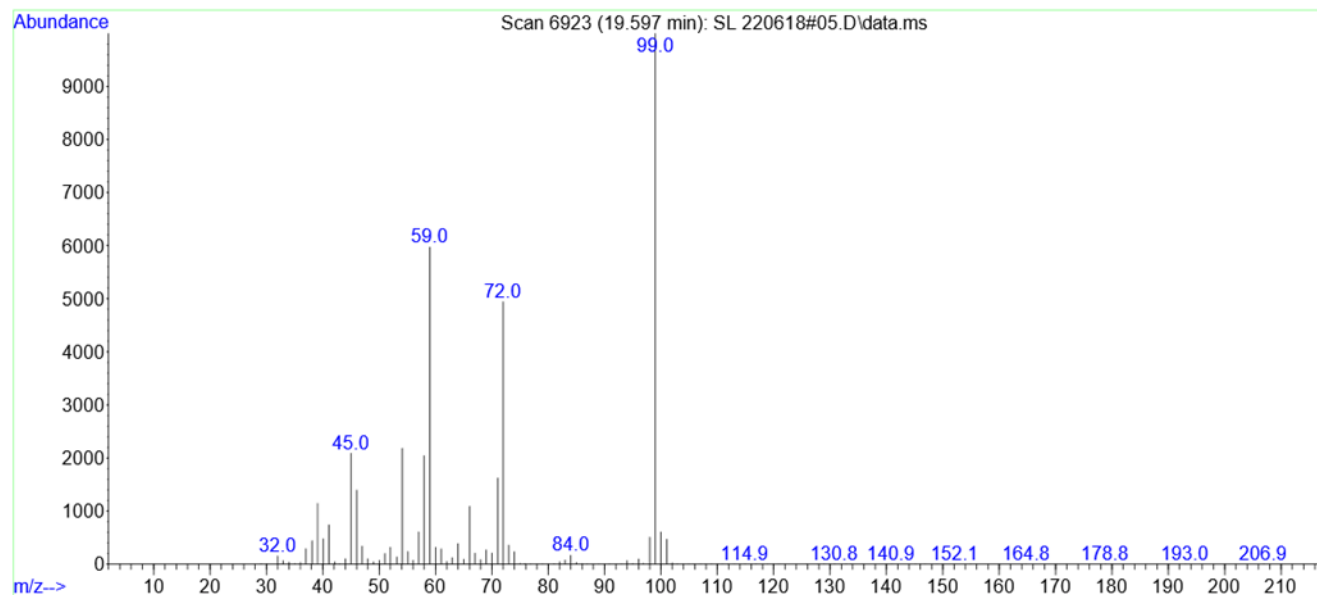
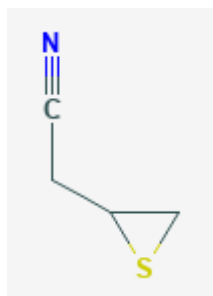
## 75. 5-methylhexanenitrile



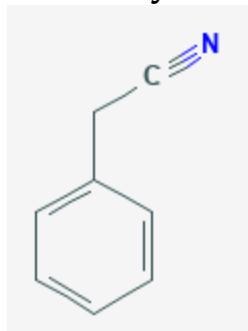
## 76. 6-heptenenitrile



## 77. Thiiraneacetonitrile



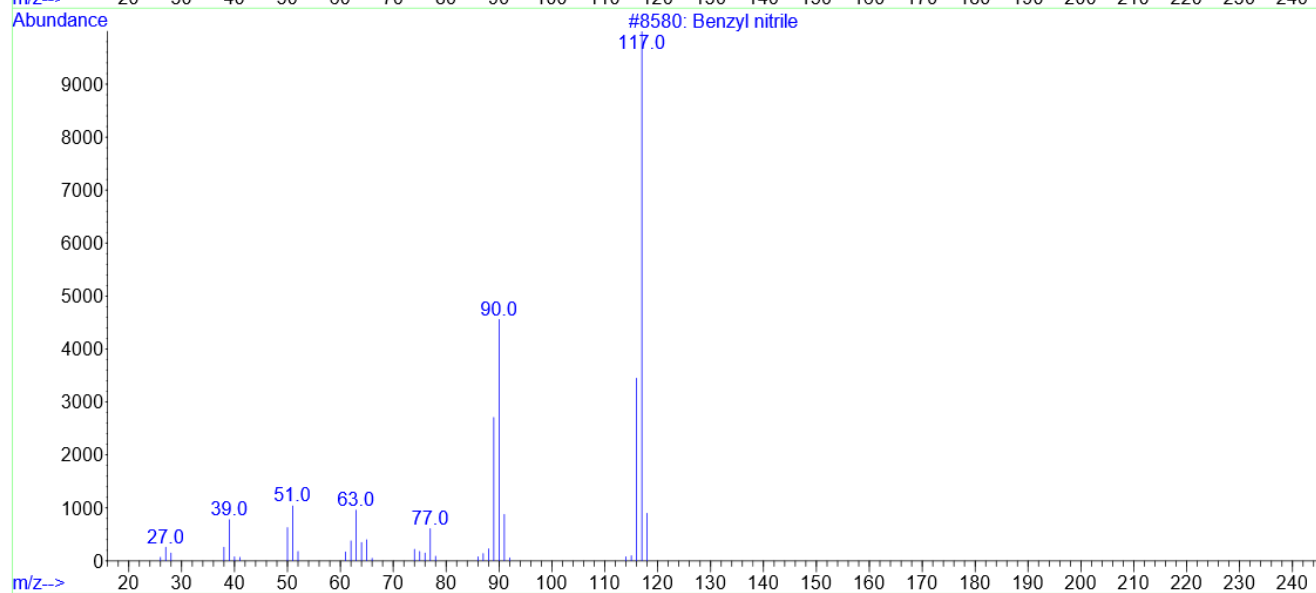
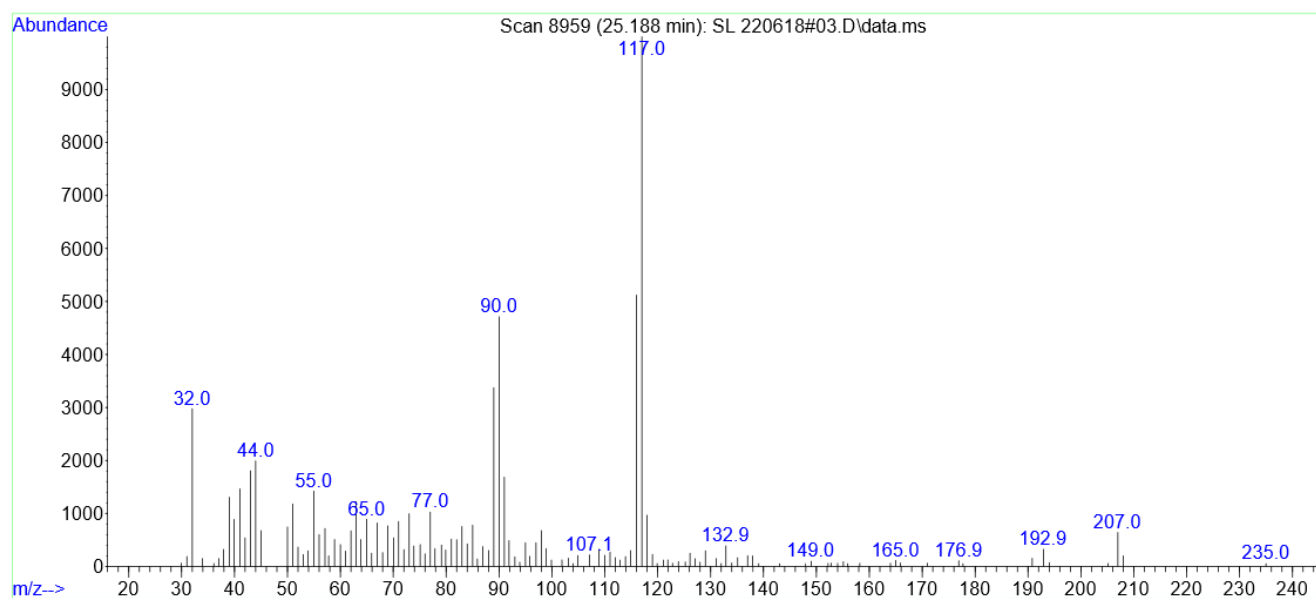
## 78. Phenylacetoneitrile



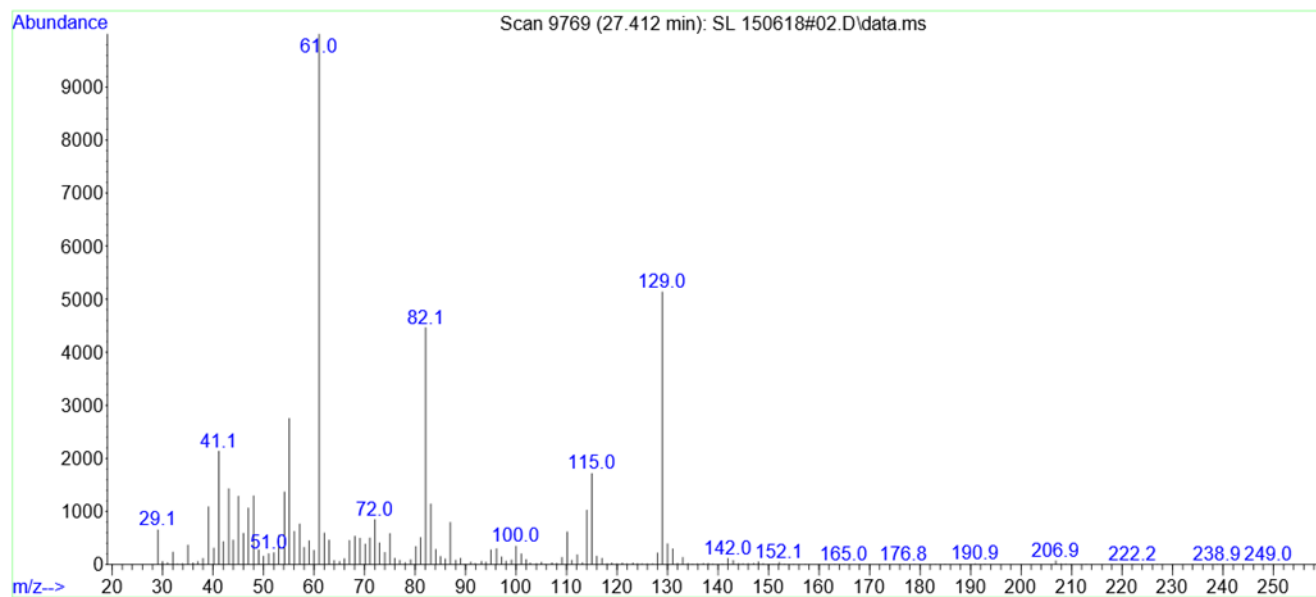
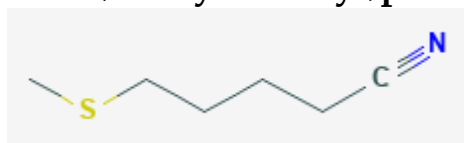
Library Searched : C:\Database\NIST11.L

Quality : 95

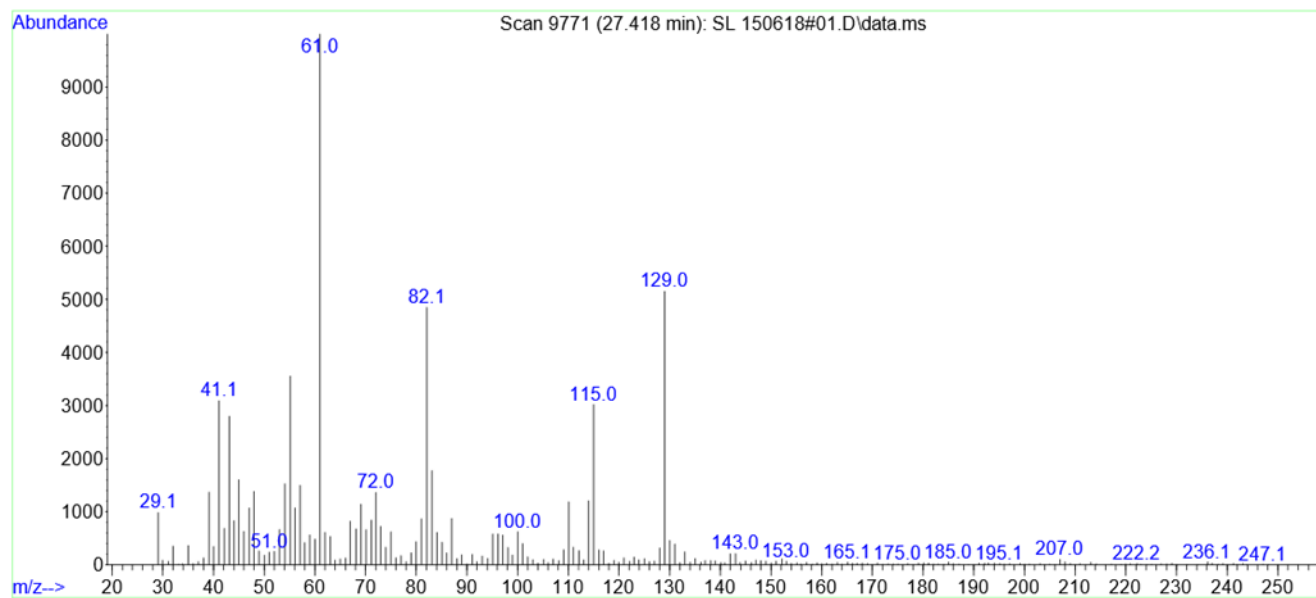
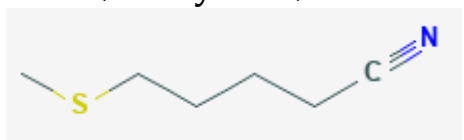
ID : Benzyl nitrile



## 79. 5-(methylsulfanyl)pentanenitrile

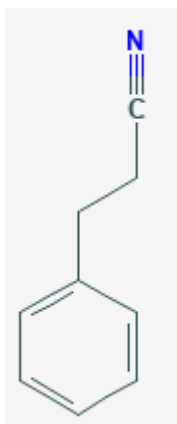


## 80. 4-(methylthio)butanenitrile





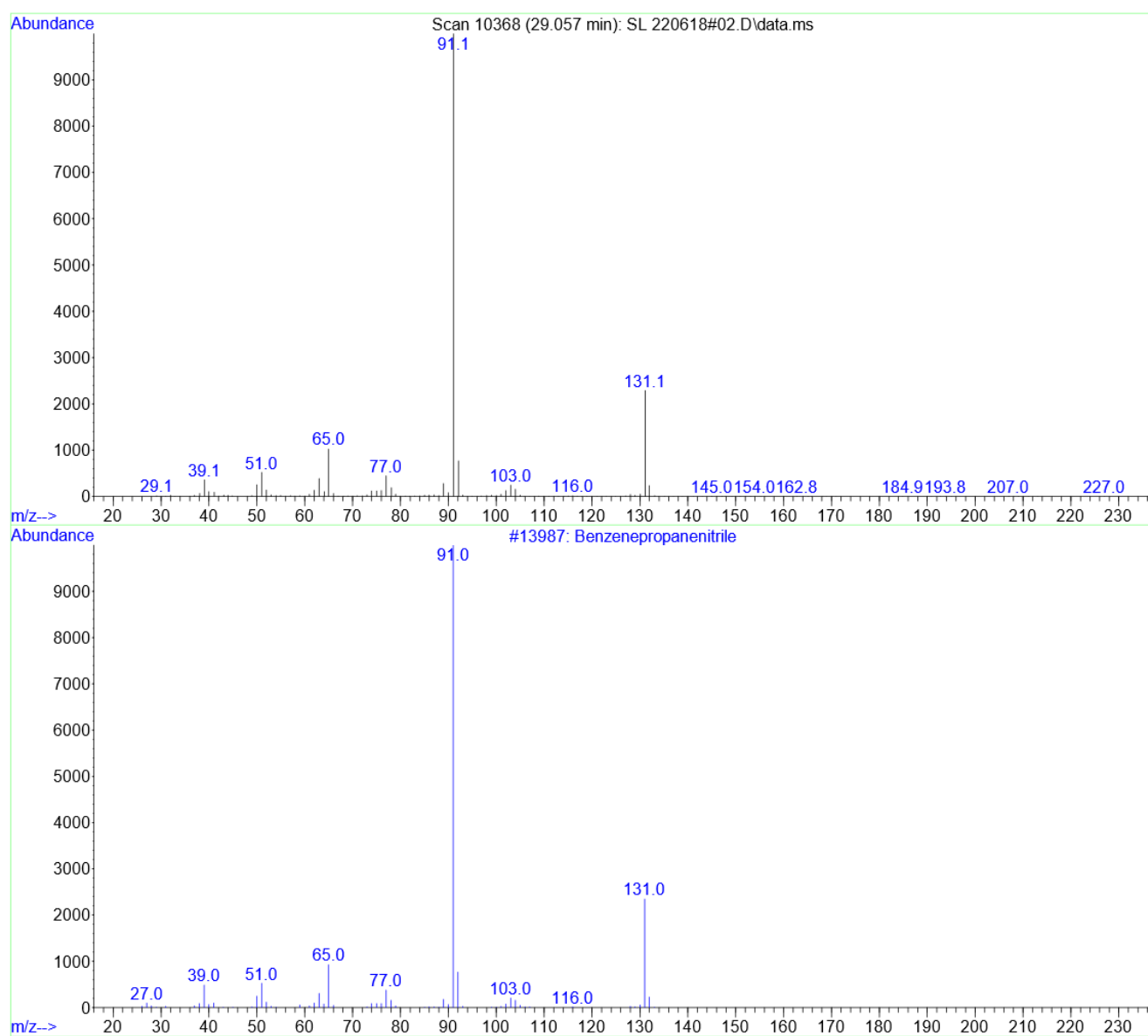
## 81. Benzenepropanenitrile



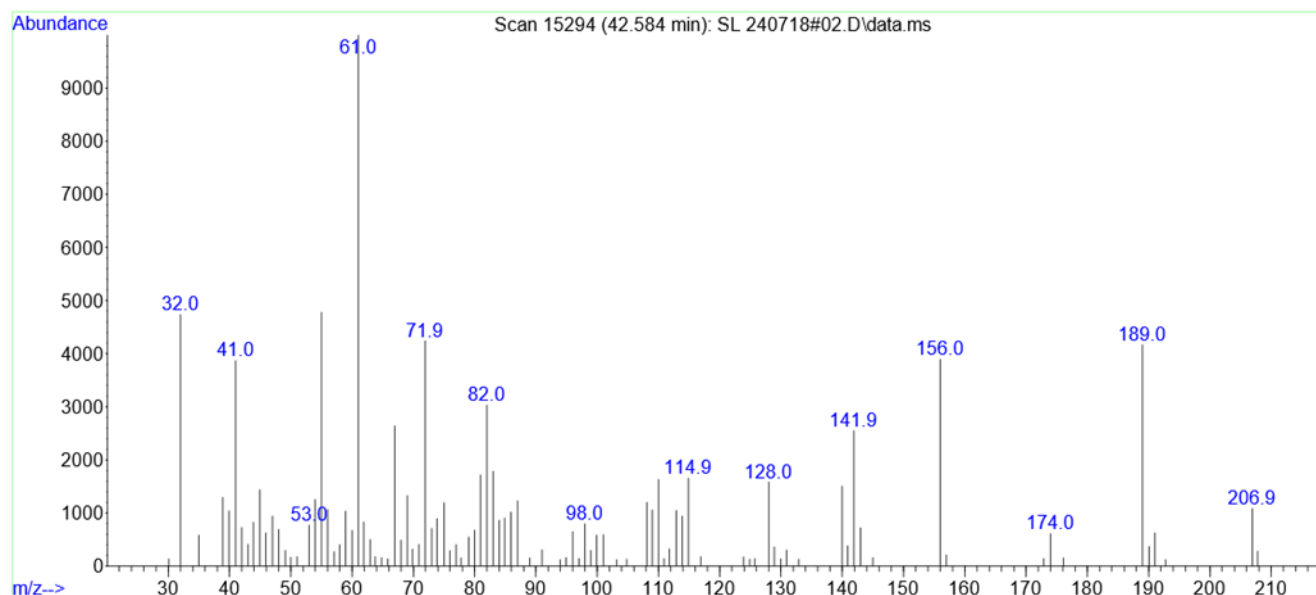
Library Searched : C:\Database\NIST11.L

Quality : 91

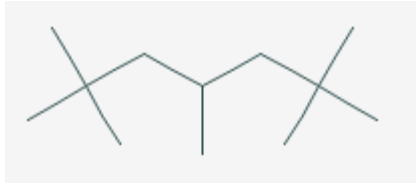
ID : Benzenepropanenitrile



## 82. unidentified nitrile



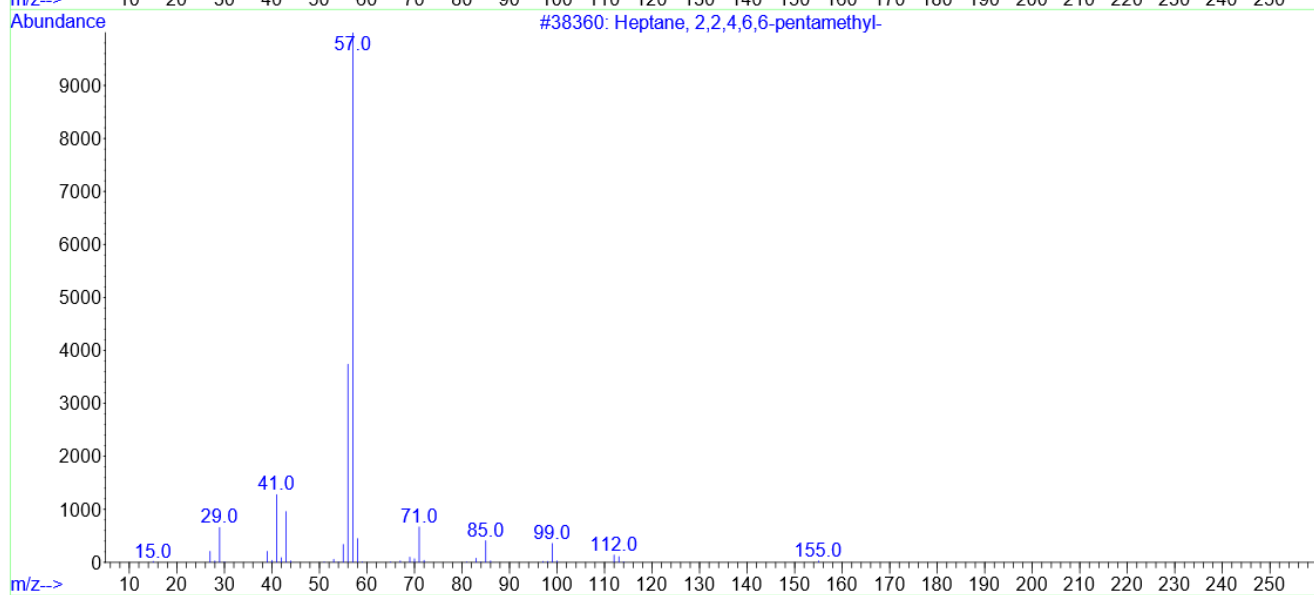
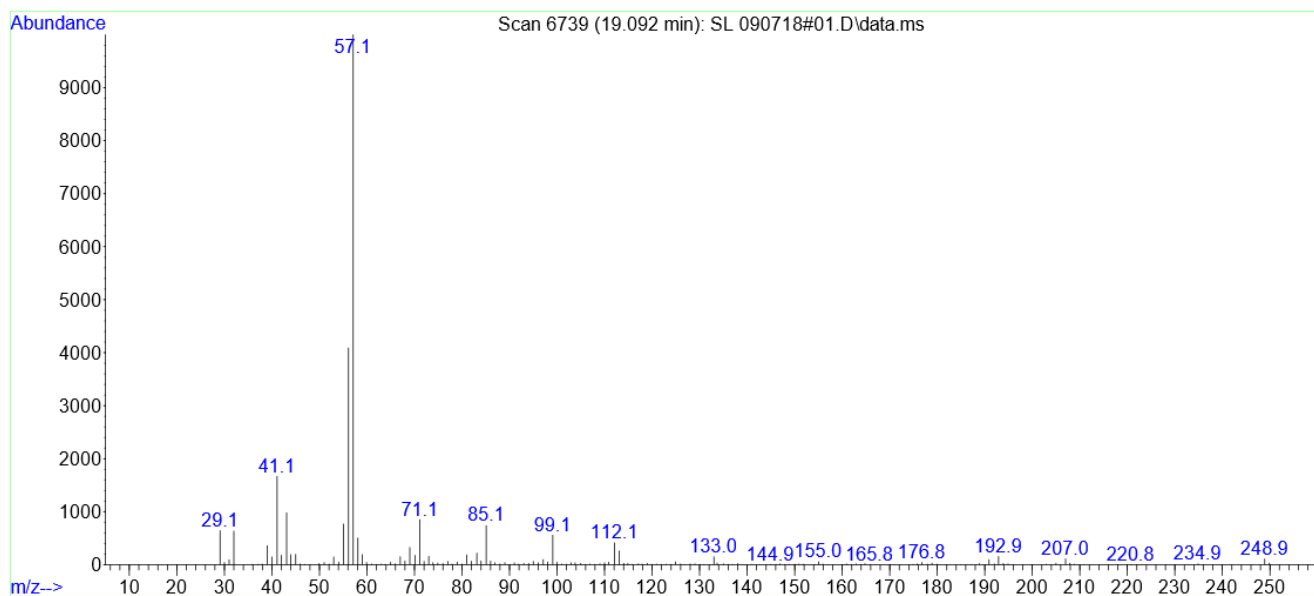
### 83. 2,2,4,6,6-pentamethylheptane



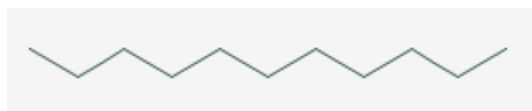
Library Searched : C:\Database\NIST11.L

Quality : 72

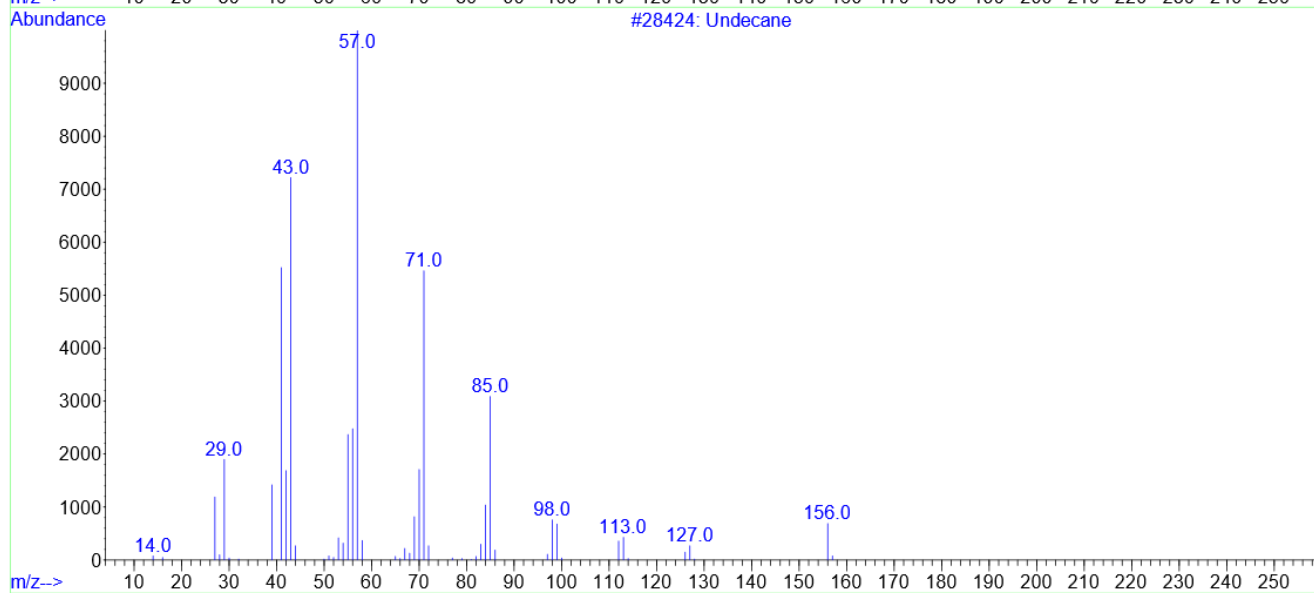
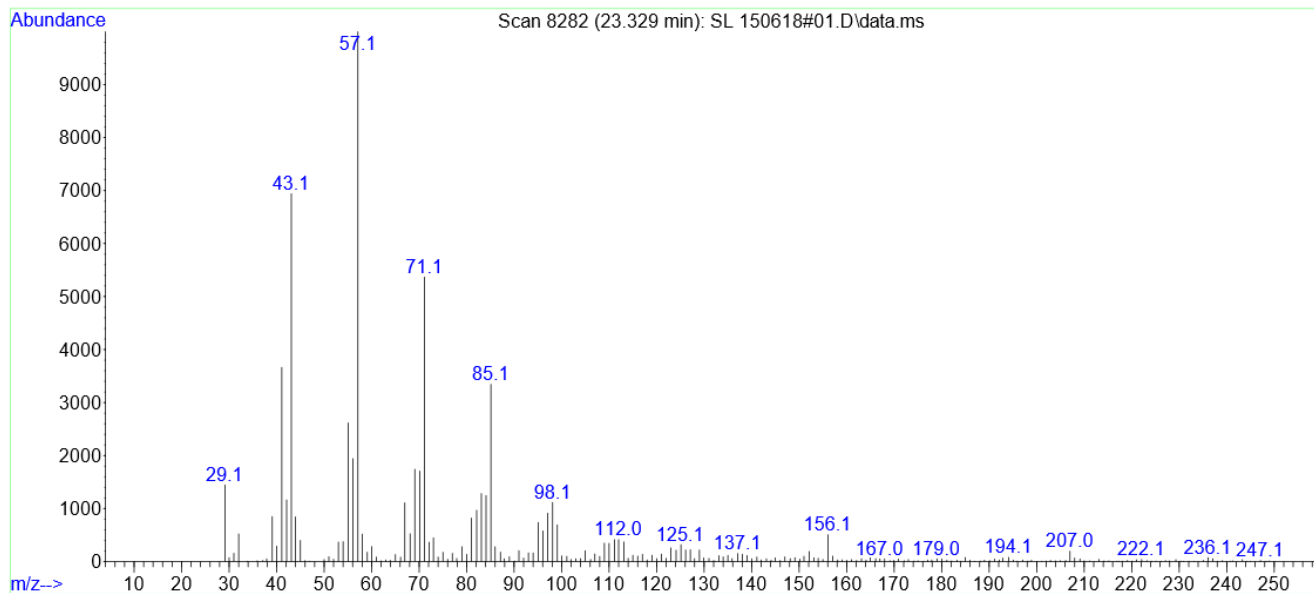
ID : Heptane, 2,2,4,6,6-pentamethyl-



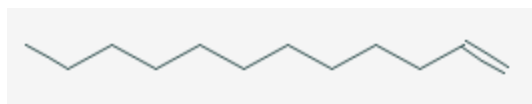
## 84. Undecane



Library Searched : C:\Database\NIST11.L  
Quality : 94  
ID : Undecane



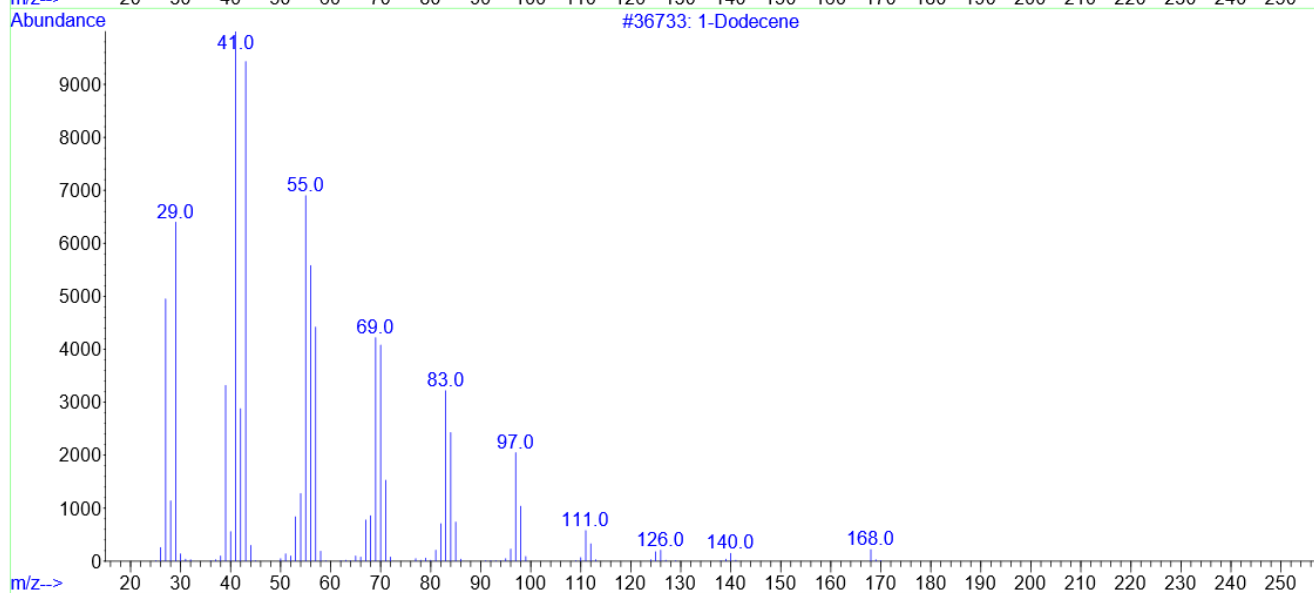
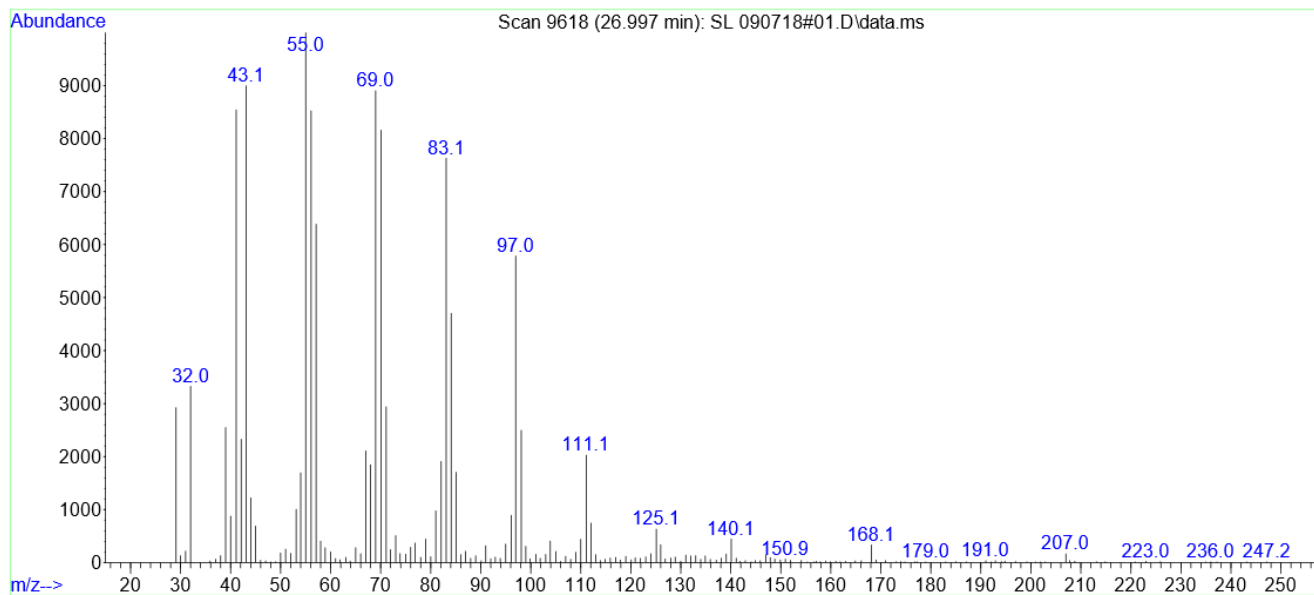
## 85. 1-dodecene



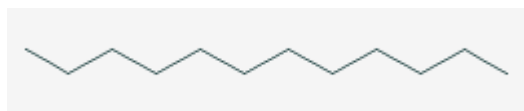
Library Searched : C:\Database\NIST11.L

Quality : 95

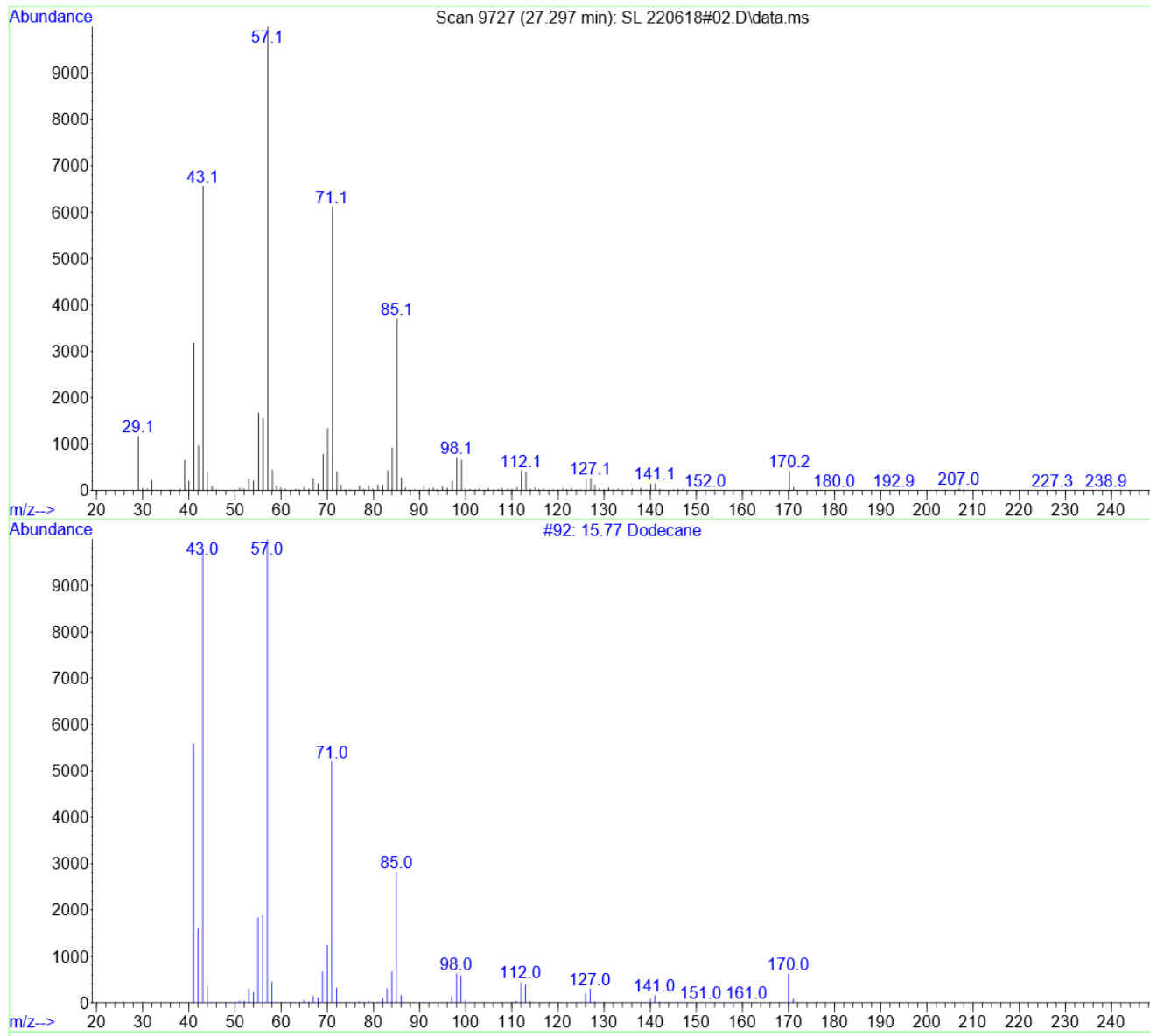
ID : 1-Dodecene



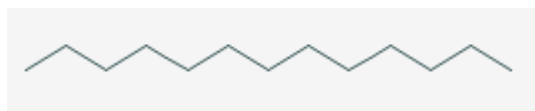
## 86. Dodecane



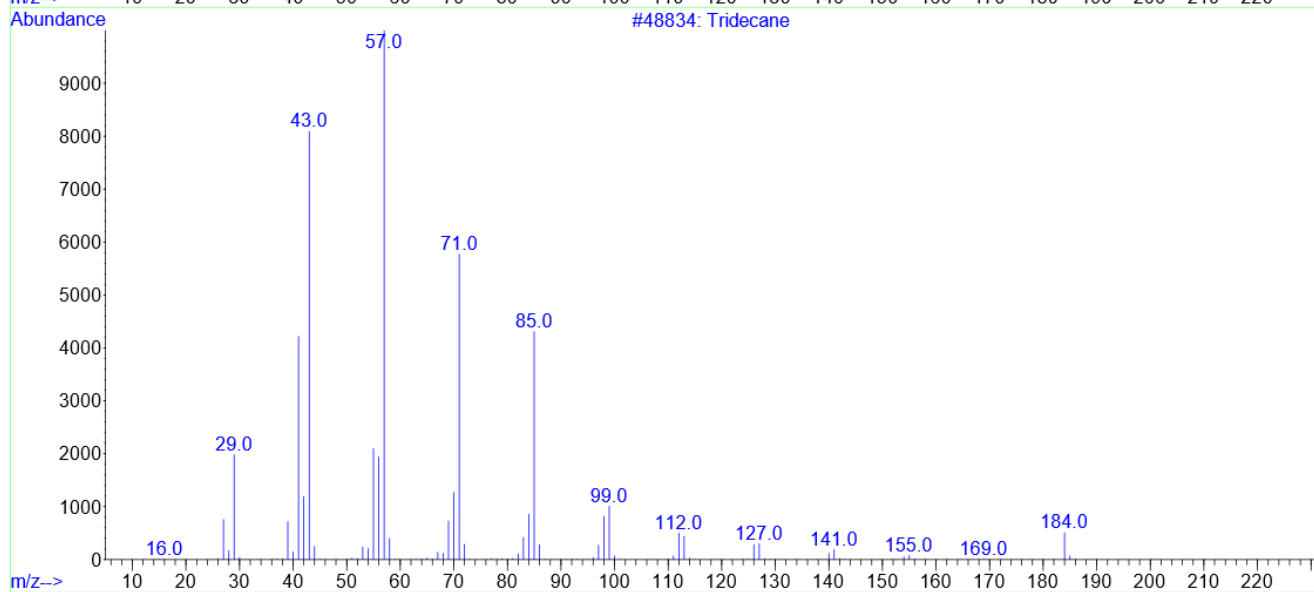
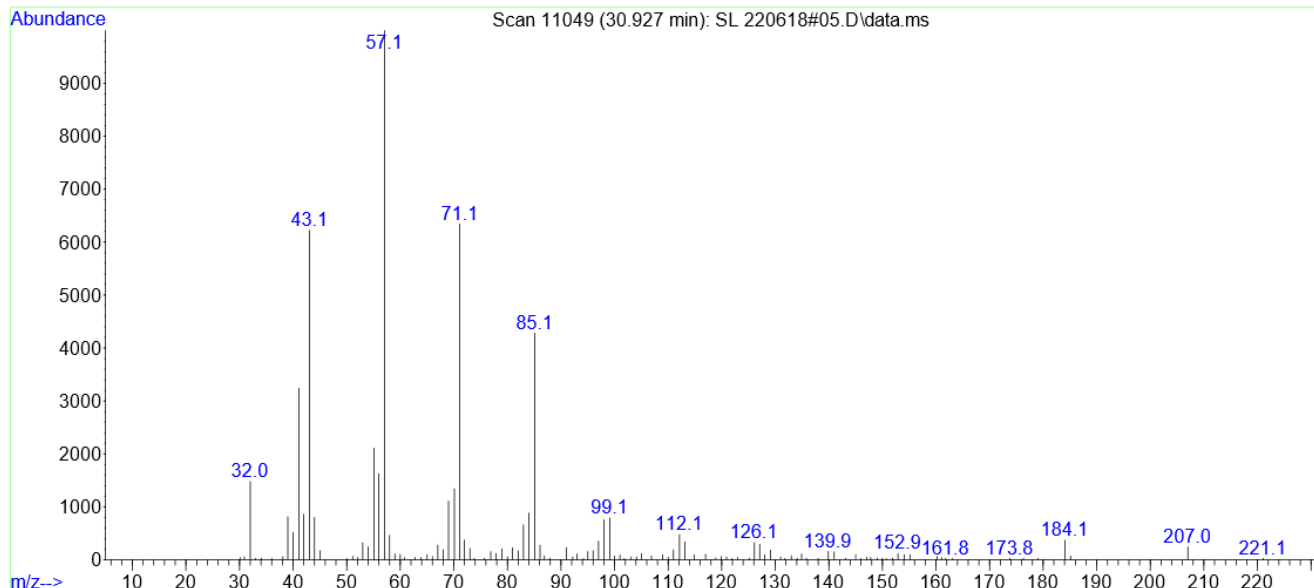
Library Searched : C:\Database\Adams.L  
Quality : 95  
ID : 15.77 Dodecane



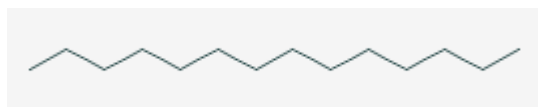
## 87. Tridecane



Library Searched : C:\Database\NIST11.L  
Quality : 96  
ID : Tridecane



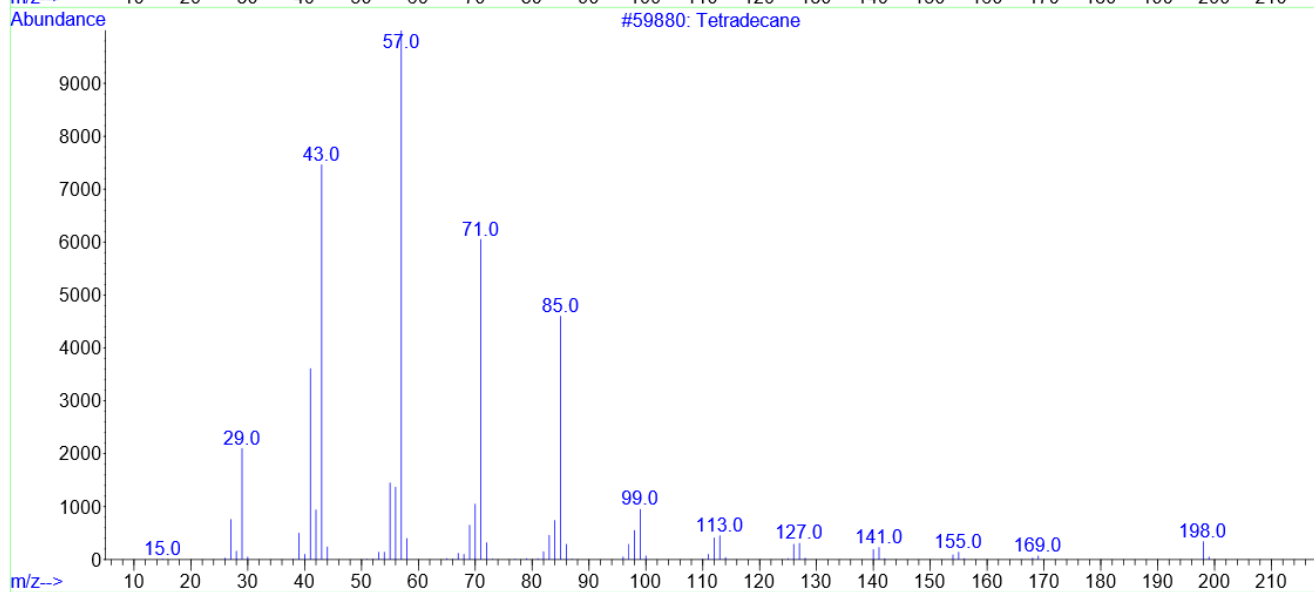
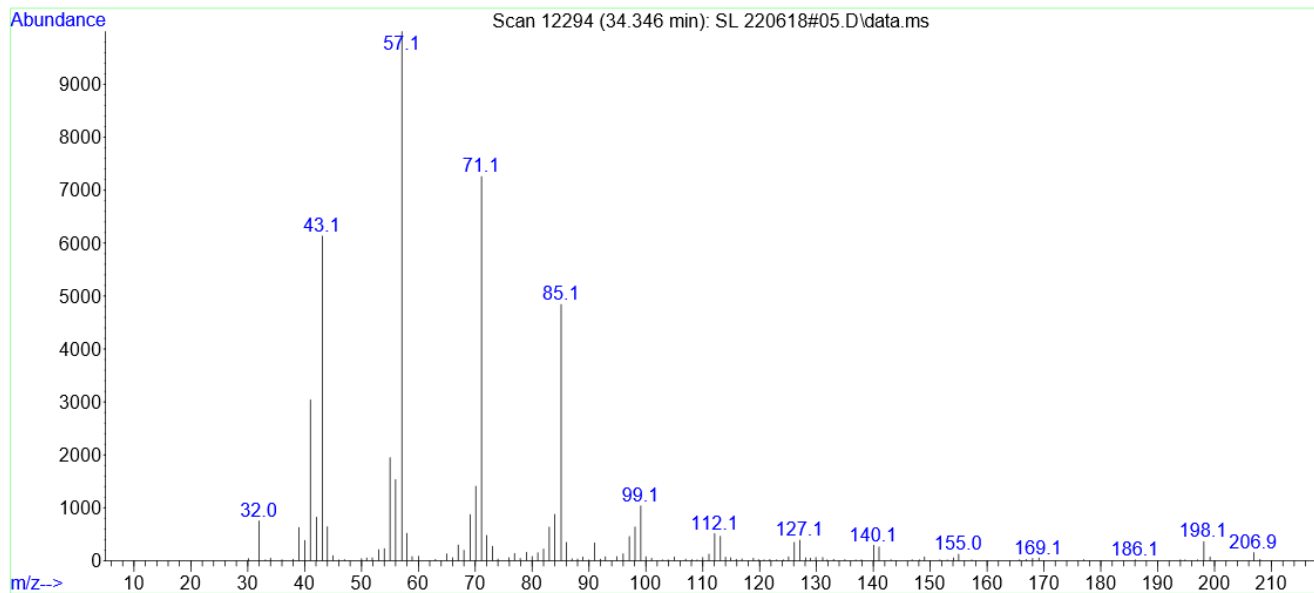
## 88. Tetradecane



Library Searched : C:\Database\NIST11.L

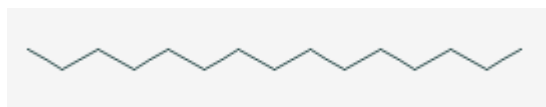
Quality : 98

ID : Tetradecane





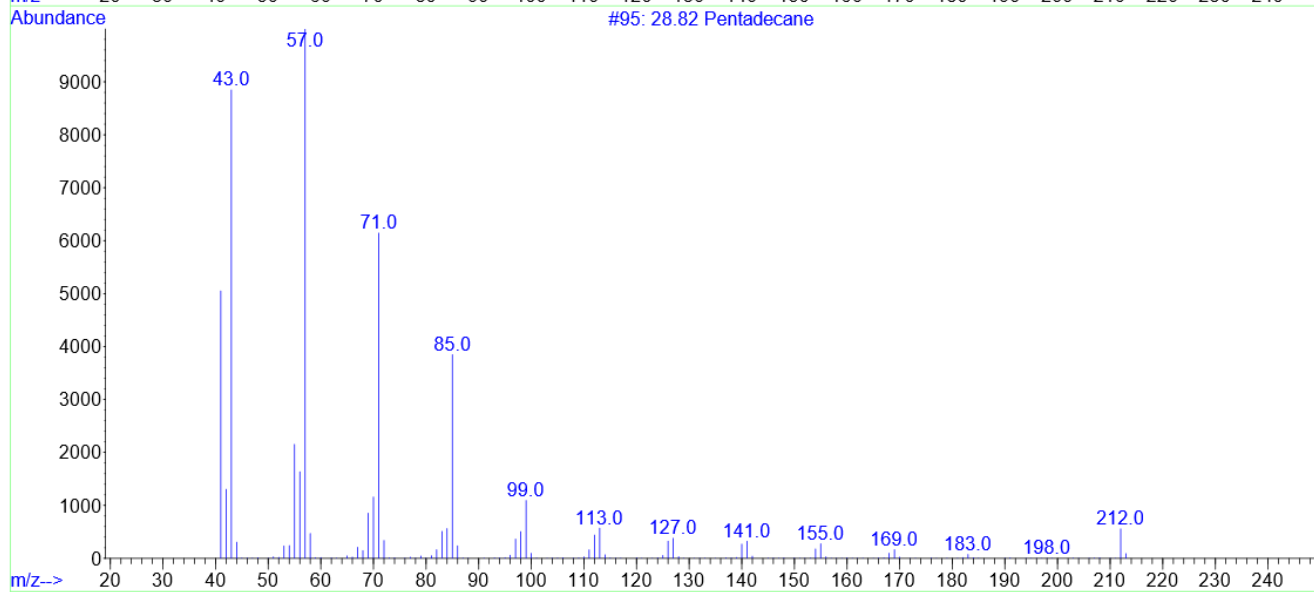
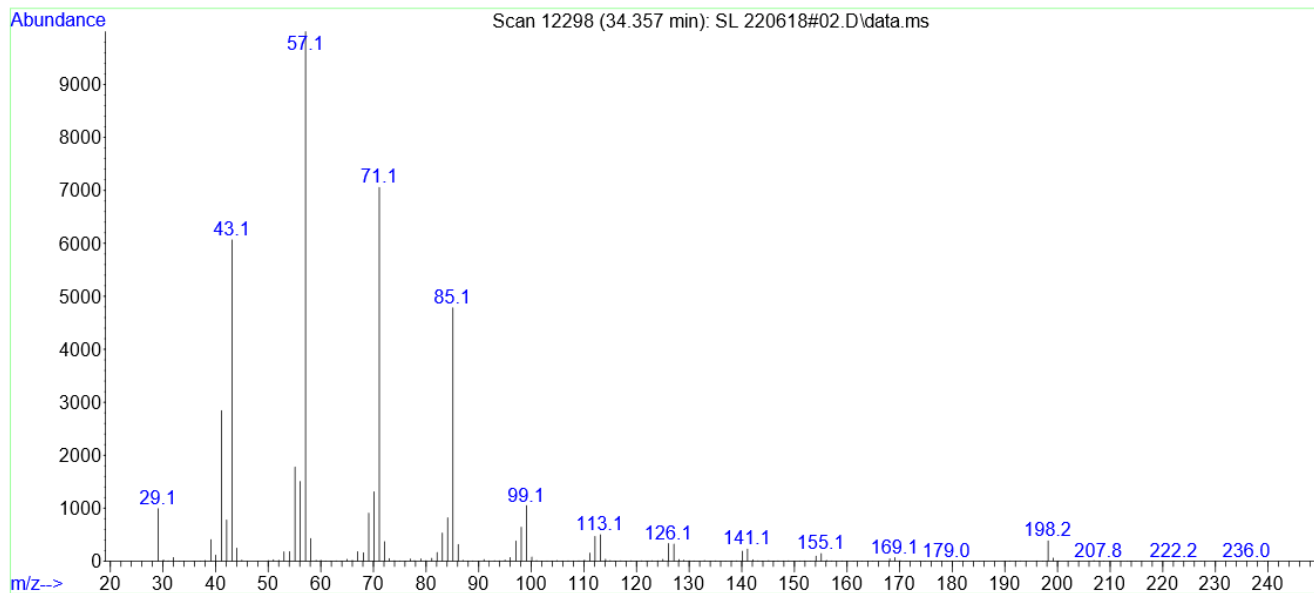
## 89. Pentadecane



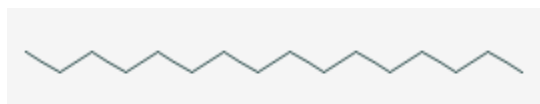
Library Searched : C:\Database\Adams.L

Quality : 90

ID : 28.82 Pentadecane



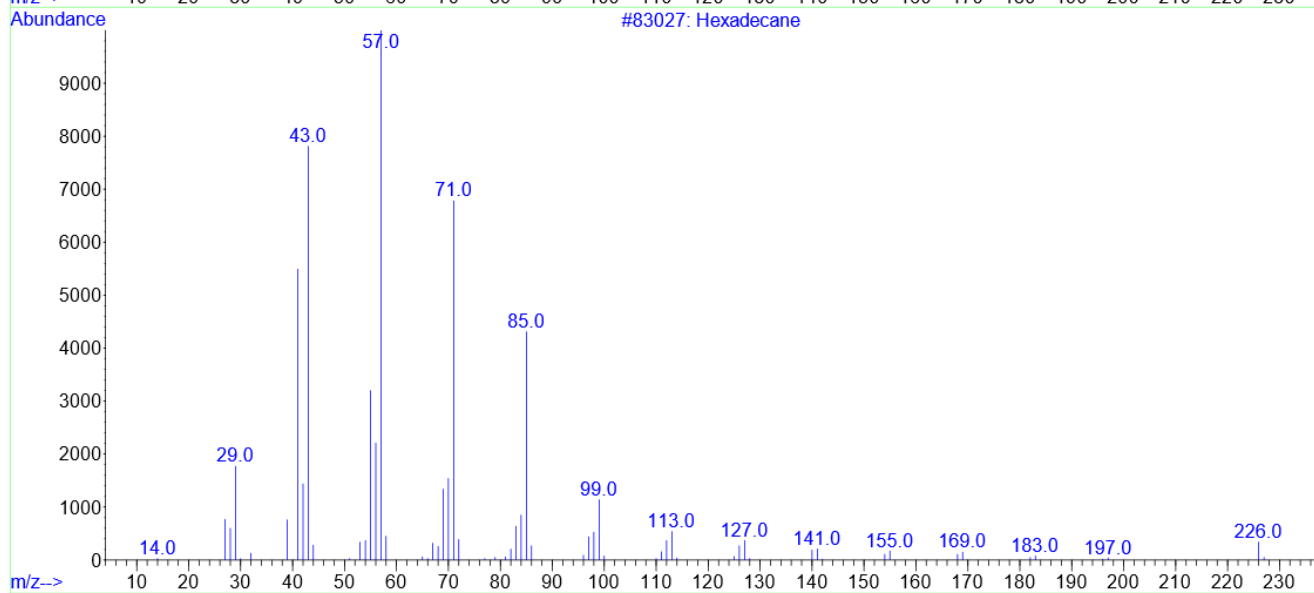
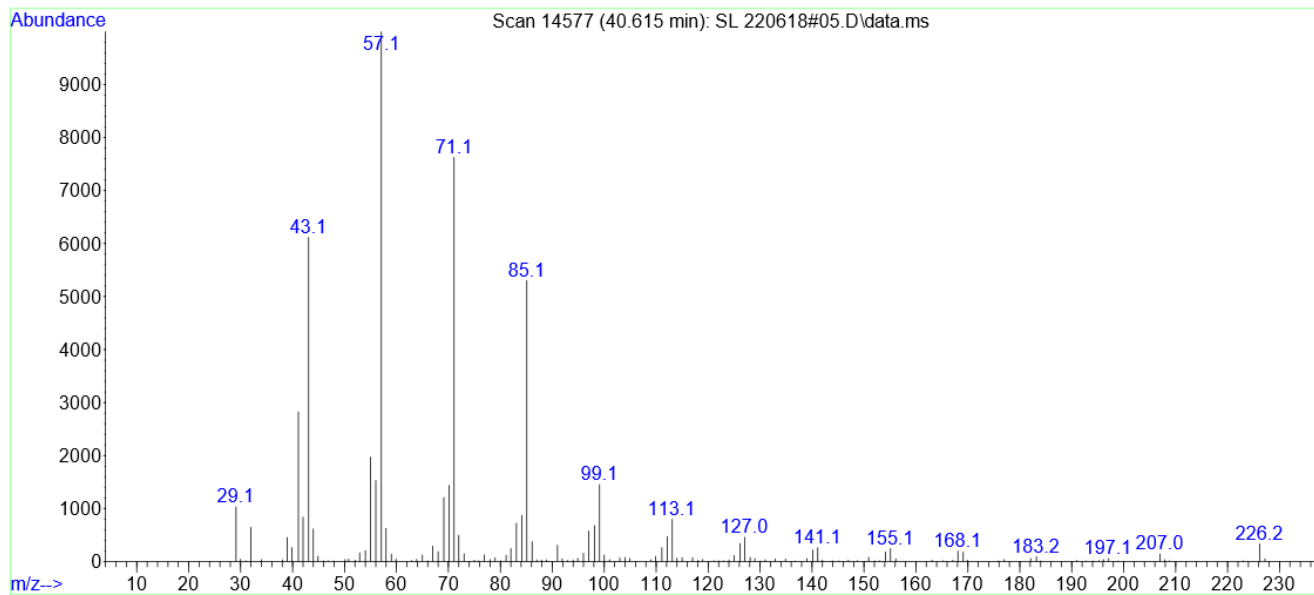
## 90. Hexadecane



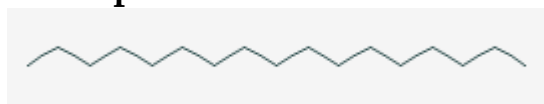
Library Searched : C:\Database\NIST11.L

Quality : 96

ID : Hexadecane



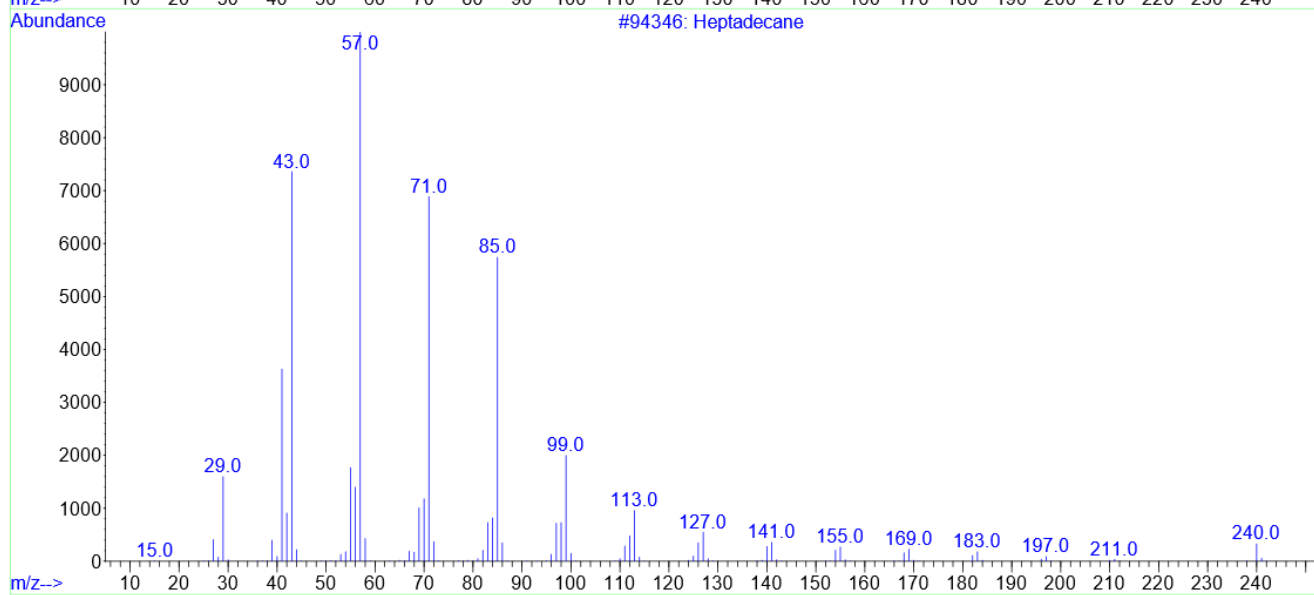
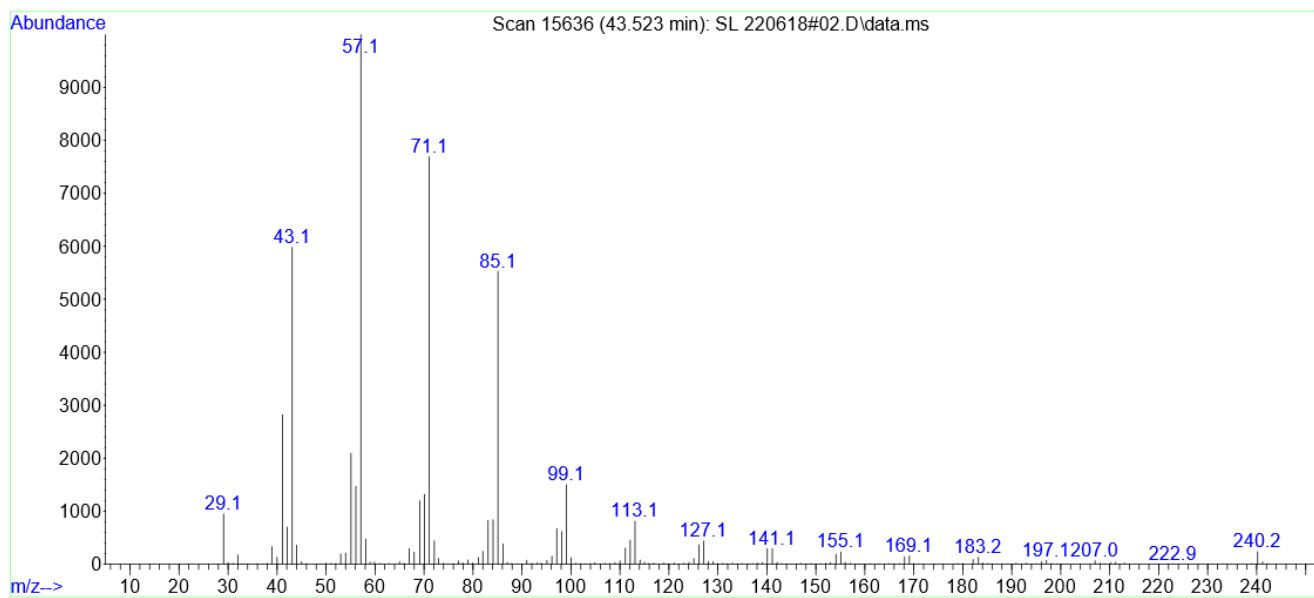
# 91. Heptadecane



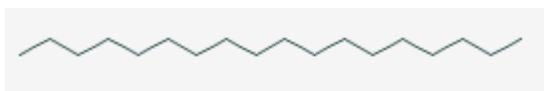
Library Searched : C:\Database\NIST11.L

Quality : 98

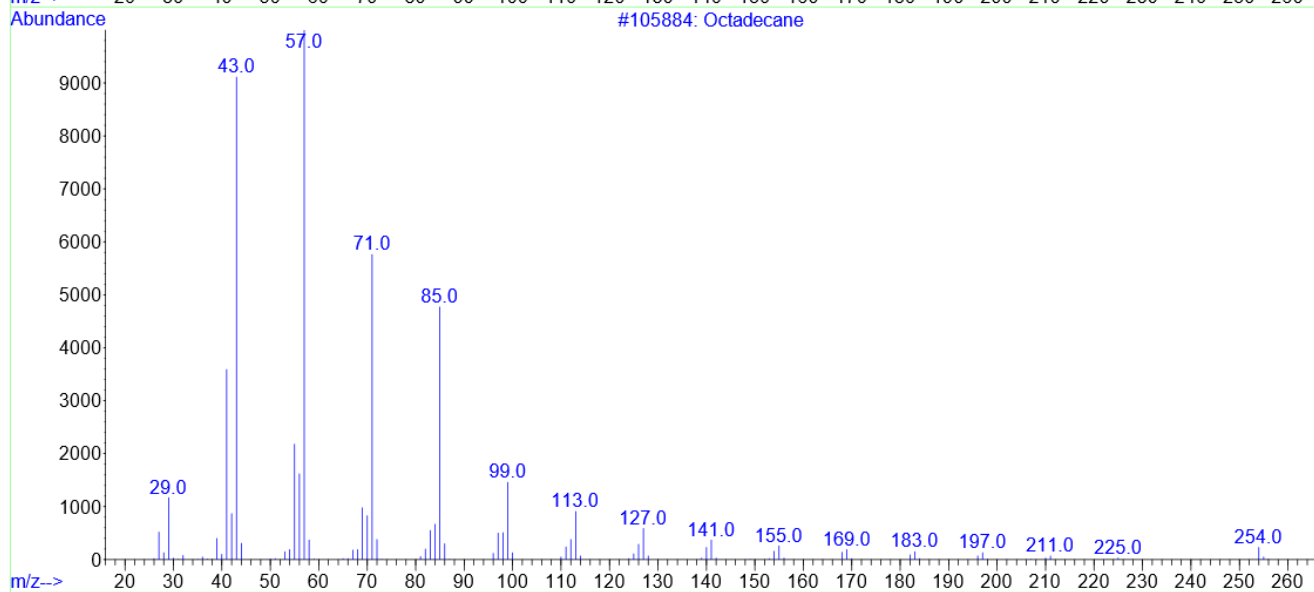
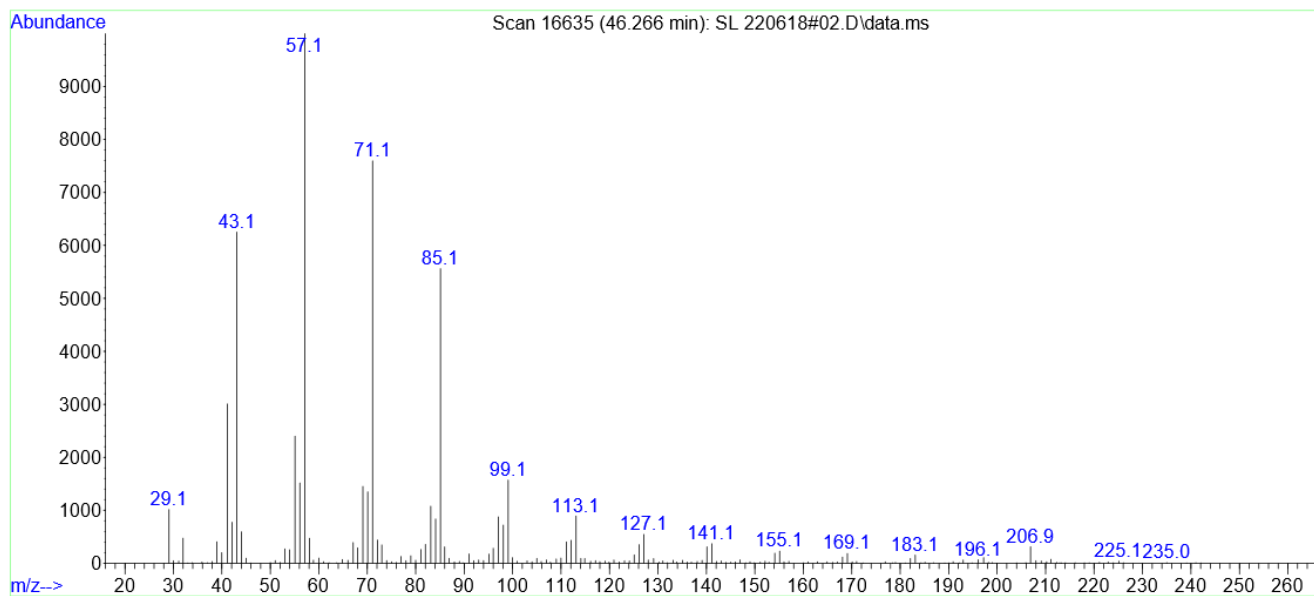
ID : Heptadecane



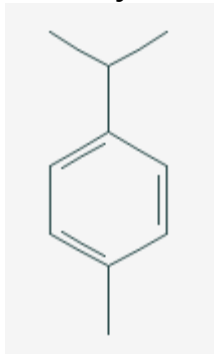
## 92. Octadecane



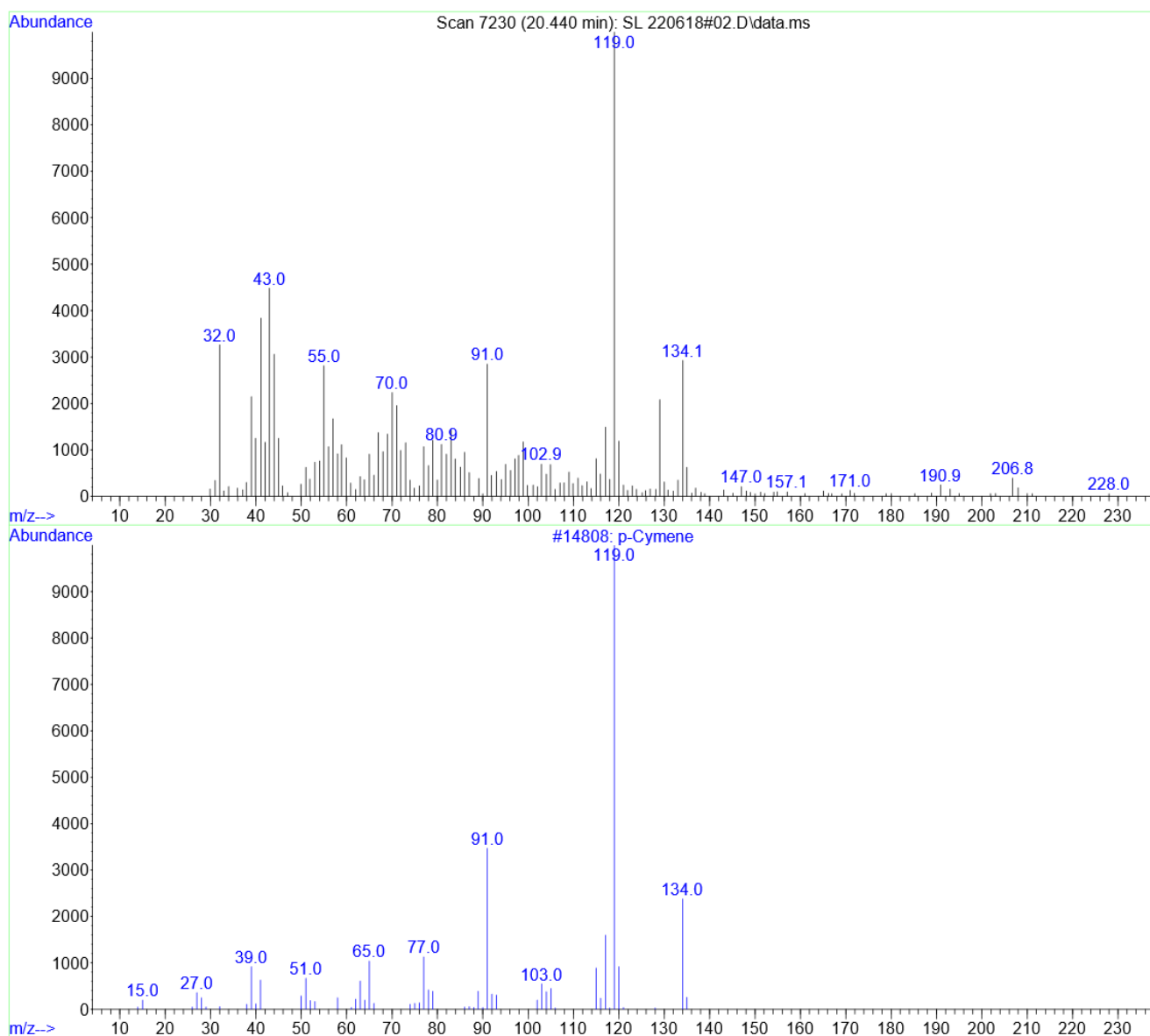
Library Searched : C:\Database\NIST11.L  
Quality : 91  
ID : Octadecane



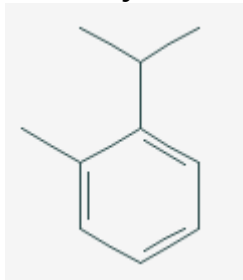
## 94. *p*-cymene



Library Searched : C:\Database\NIST11.L  
Quality : 92  
ID : *p*-Cymene



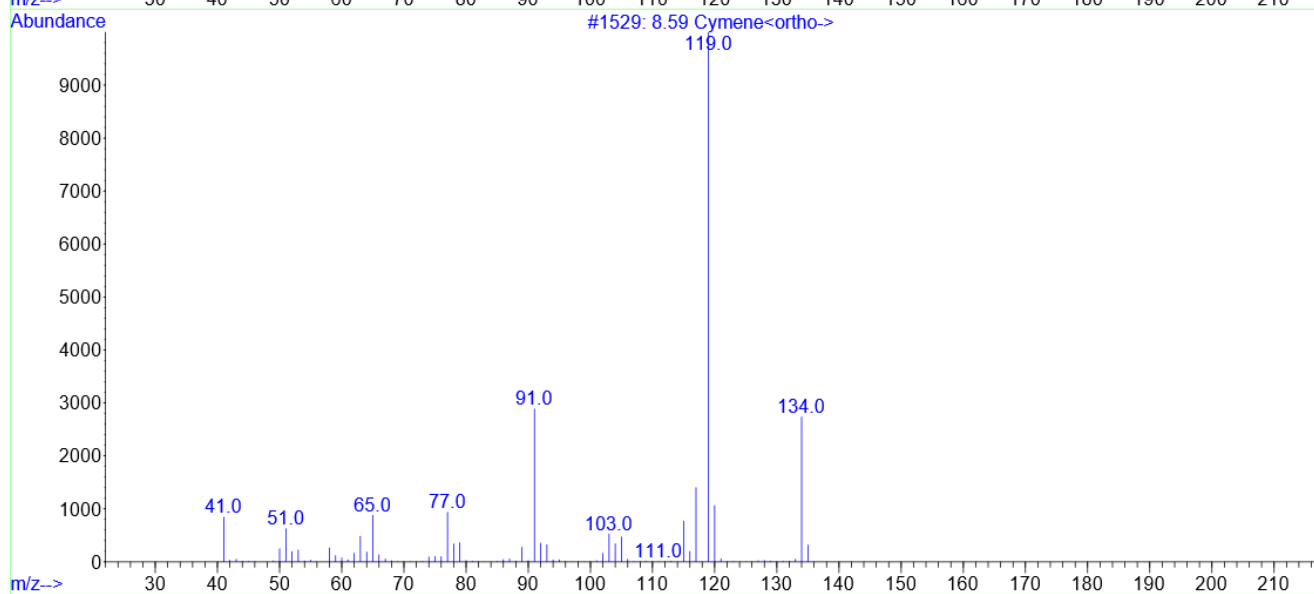
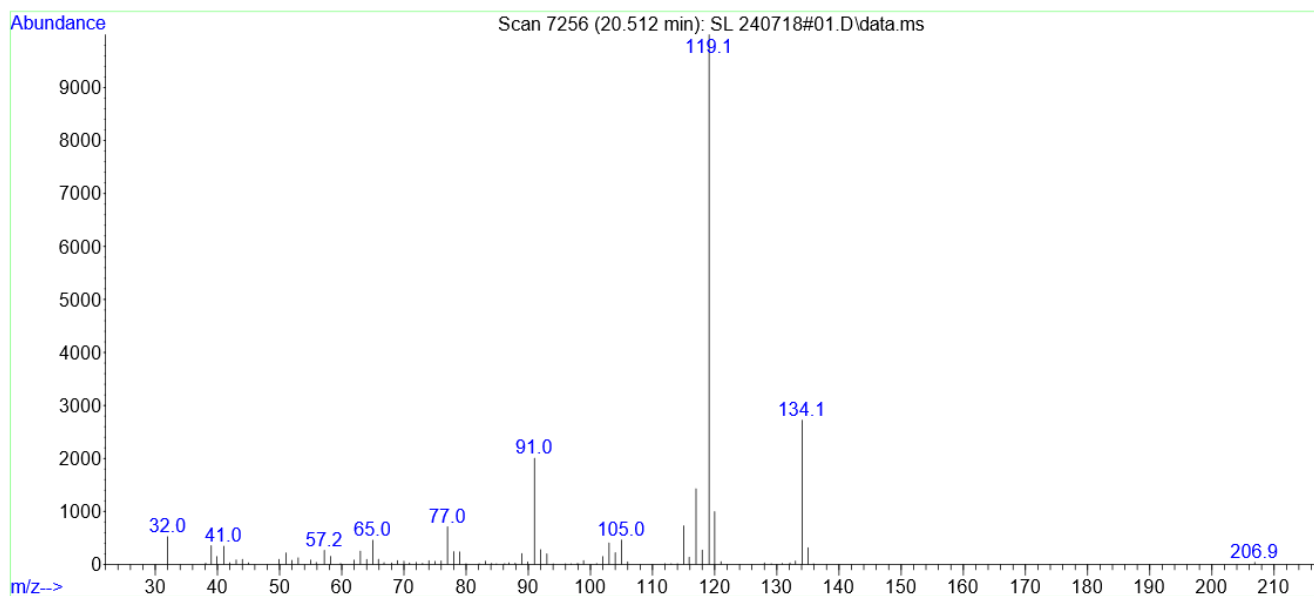
## 95. *O*-cymene



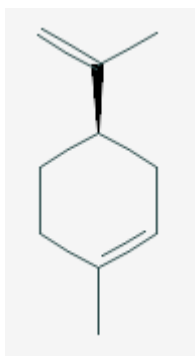
Library Searched : C:\Database\Adams.L

Quality : 95

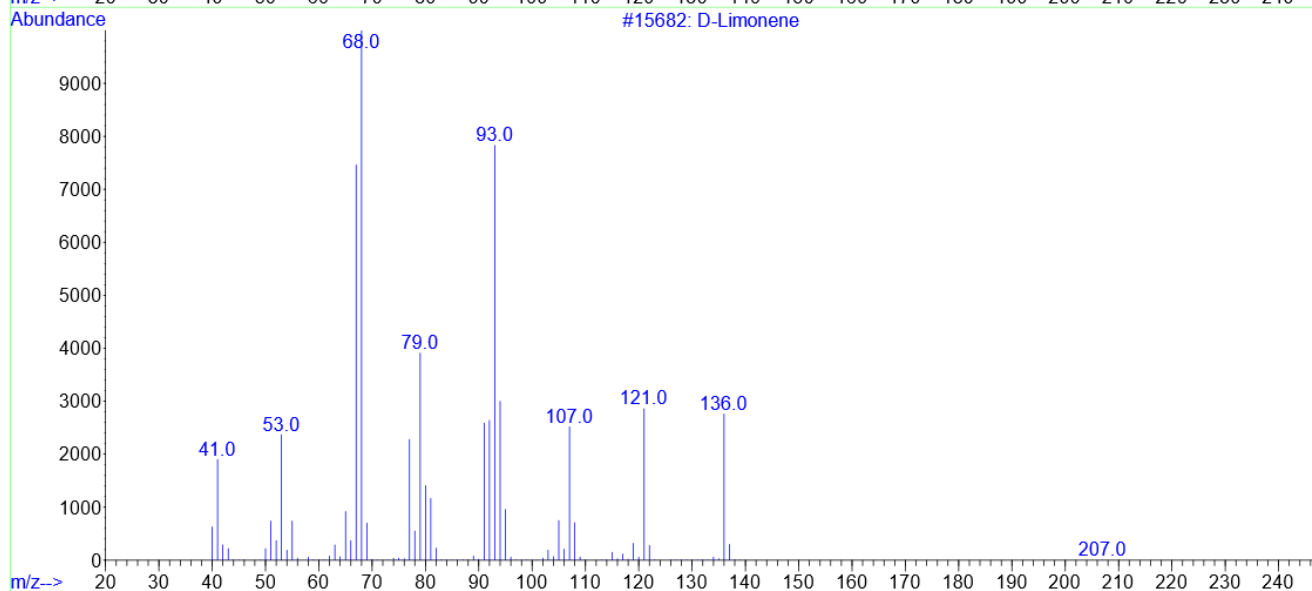
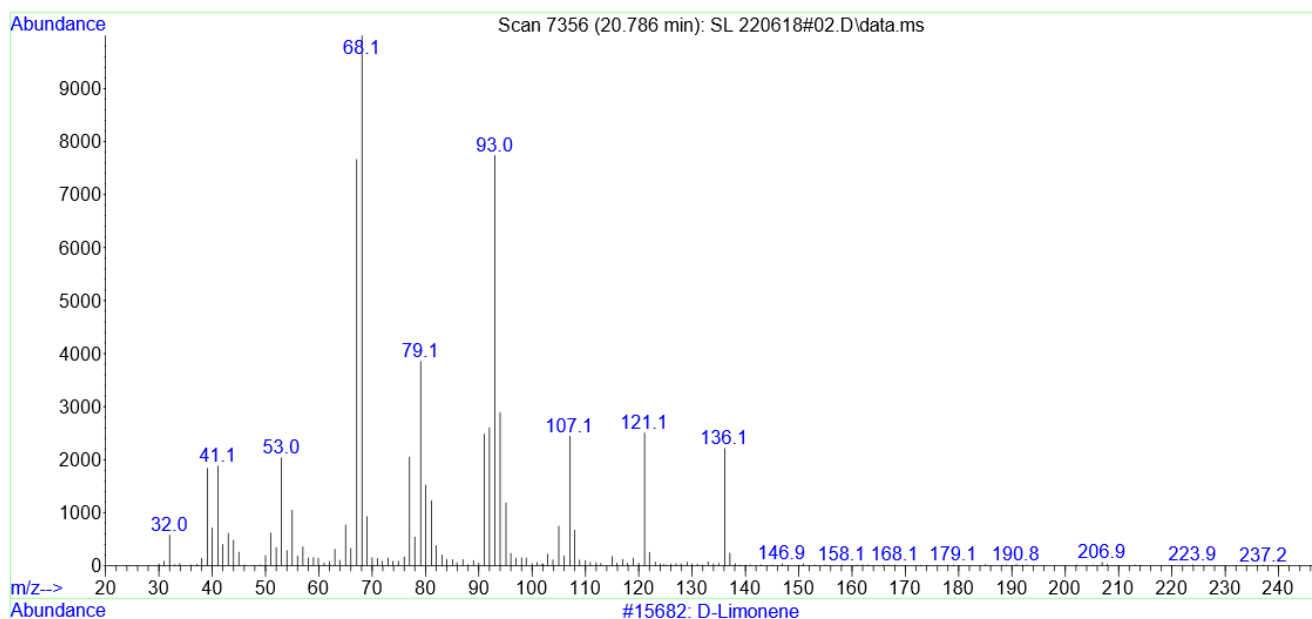
ID : 8.59 Cymene<ortho->



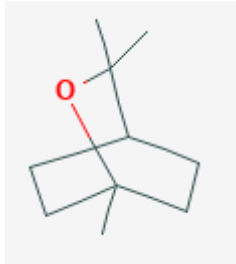
## 96. *D*-limonene



Library Searched : C:\Database\NIST11.L  
Quality : 99  
ID : D-Limonene



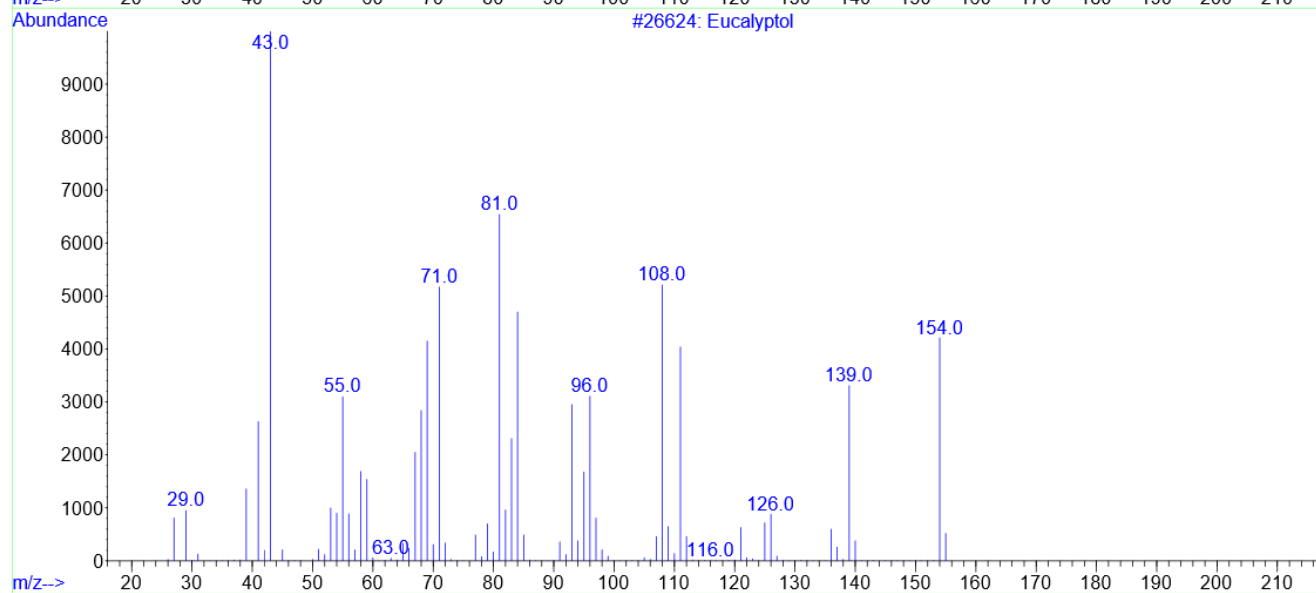
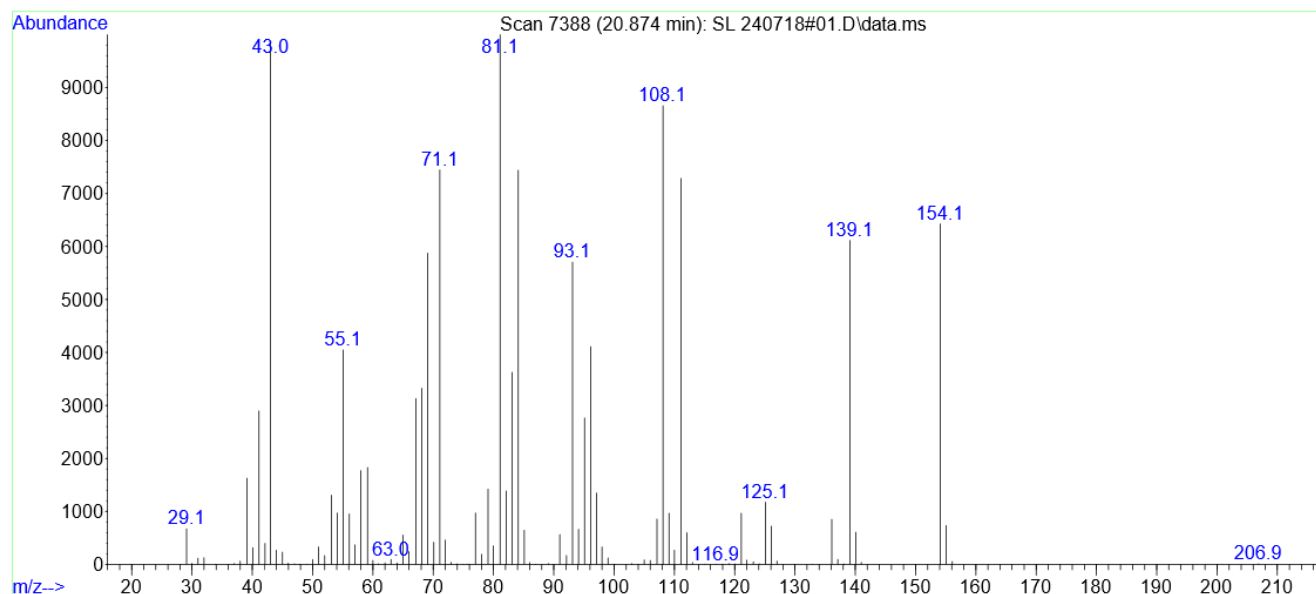
## 97. Eucalyptol



Library Searched : C:\Database\NIST11.L

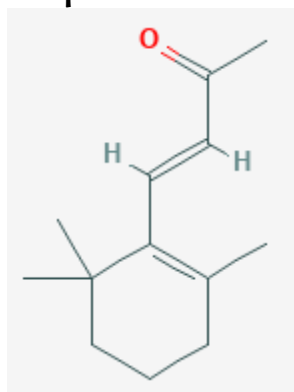
Quality : 98

ID : Eucalyptol





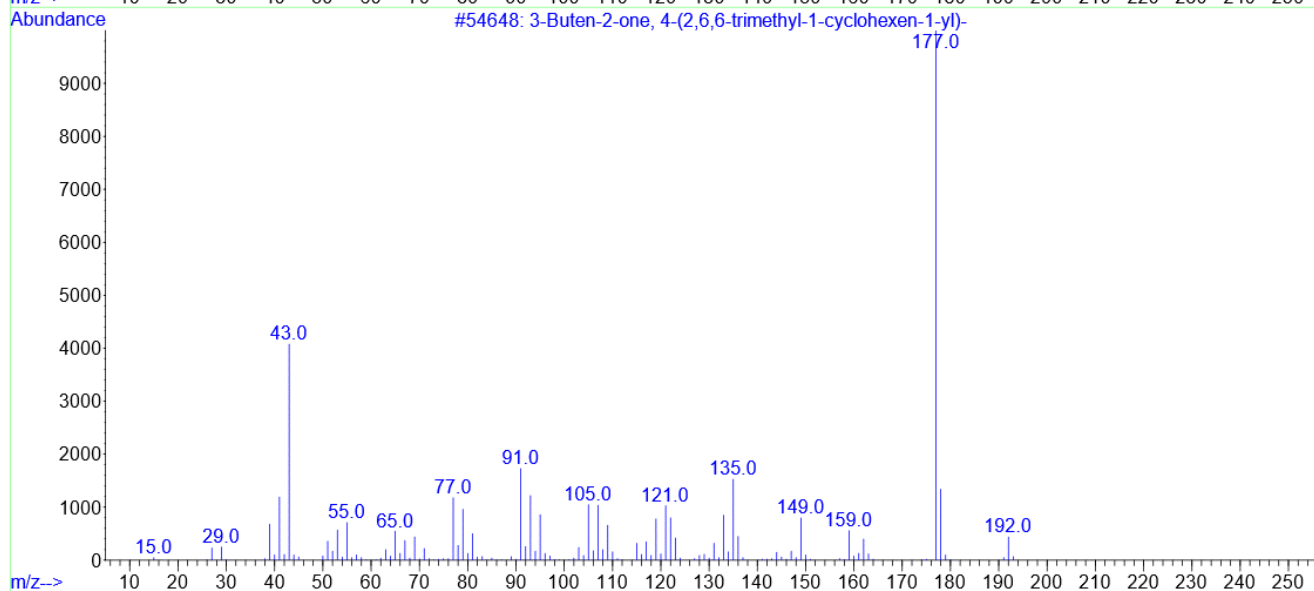
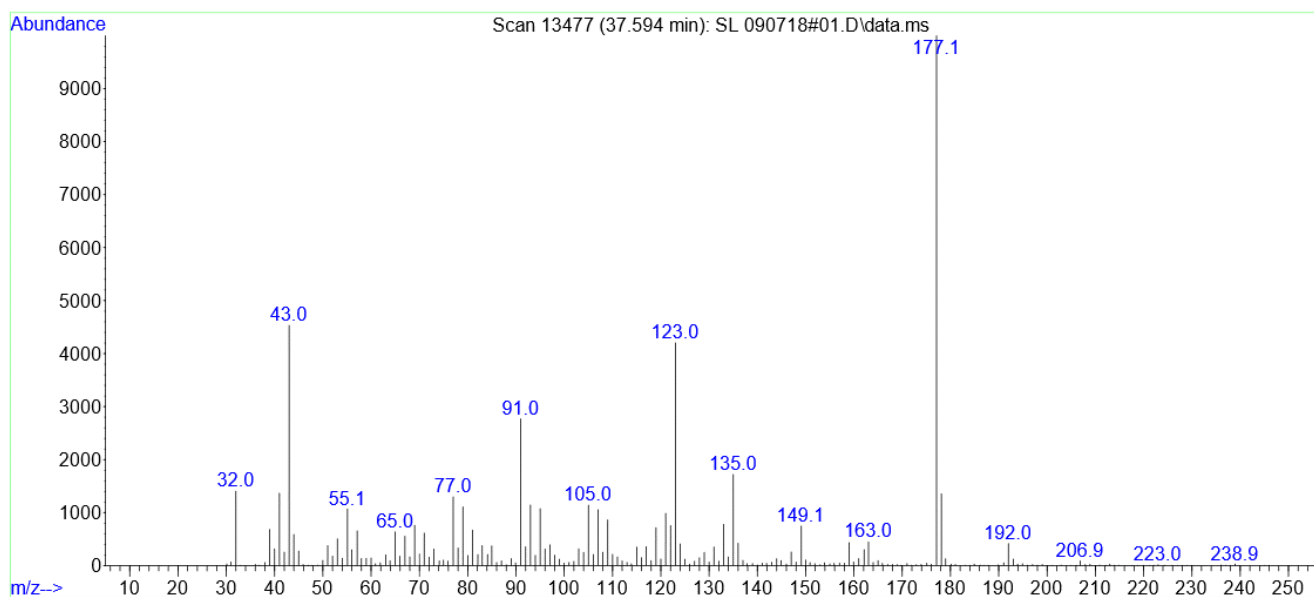
## 98. $\beta$ -ionone



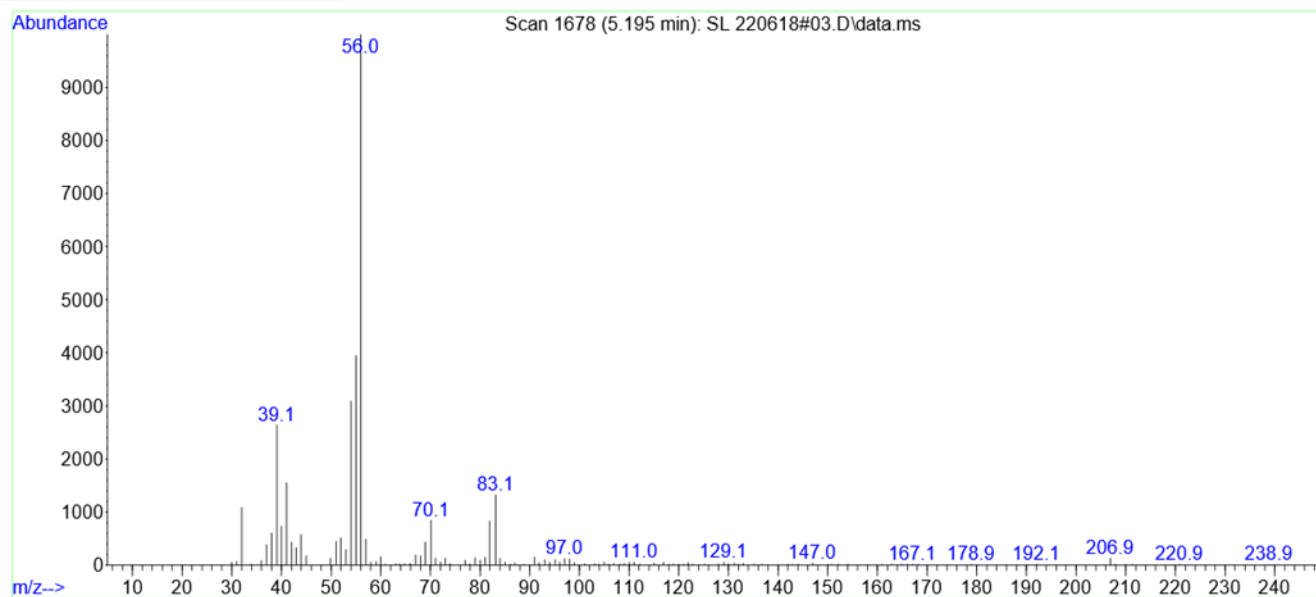
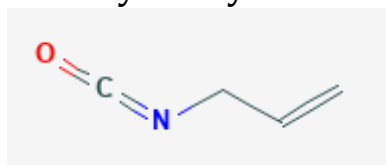
Library Searched : C:\Database\NIST11.L

Quality : 97

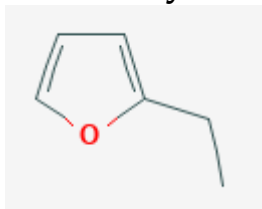
ID : 3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-



## 99. Allyl isocyanate



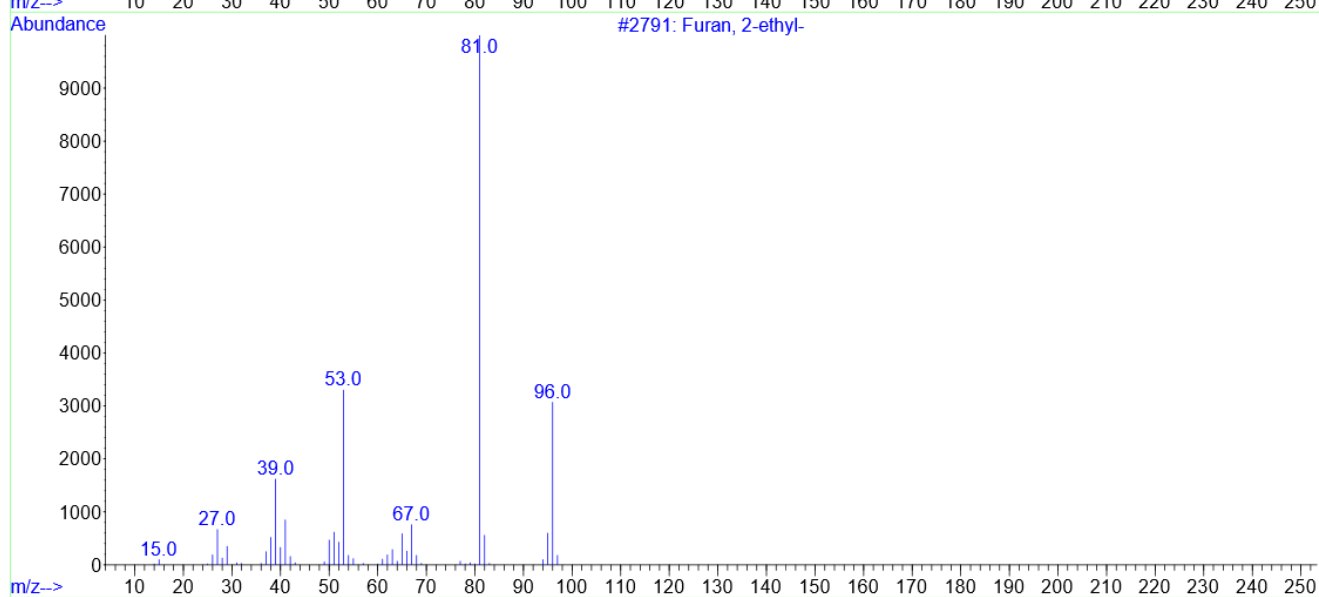
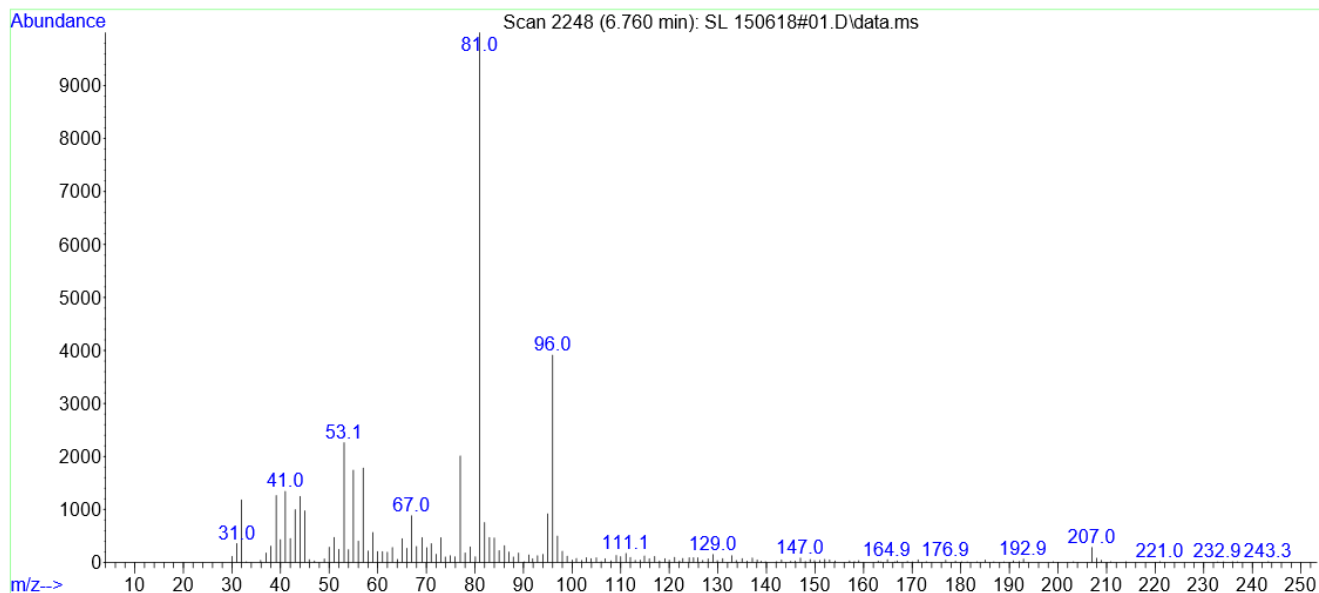
## 100. 2-ethylfuran



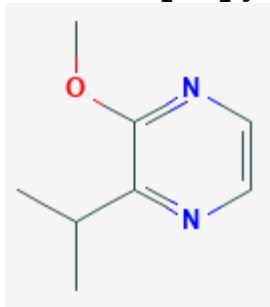
Library Searched : C:\Database\NIST11.L

Quality : 76

ID : Furan, 2-ethyl-



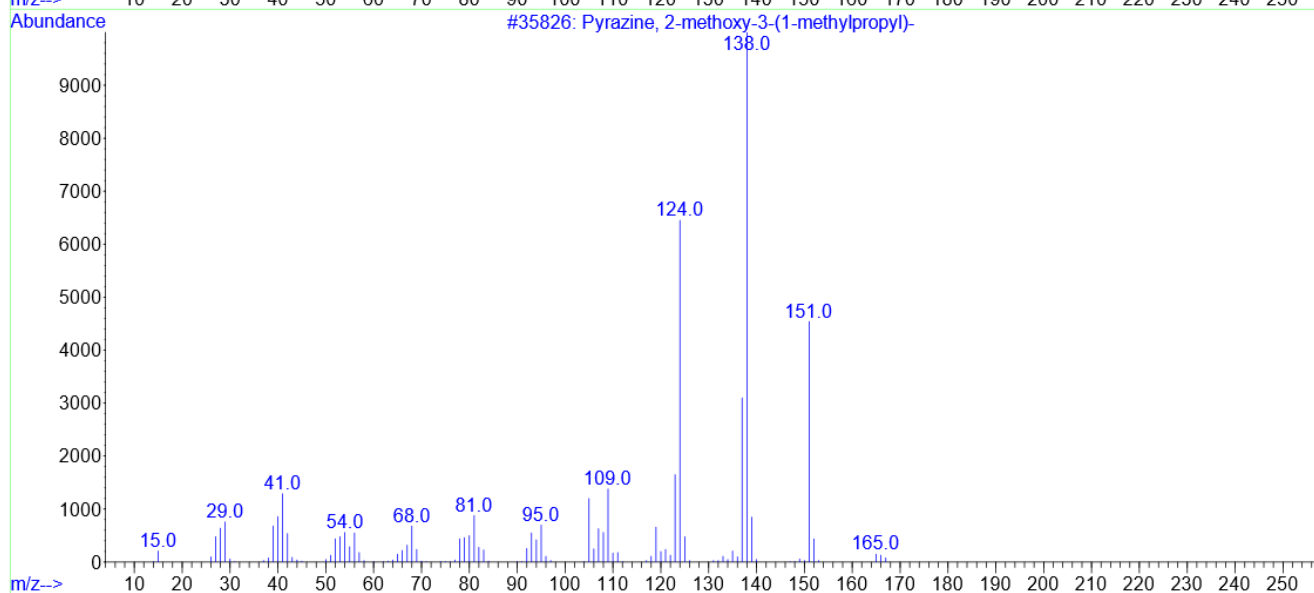
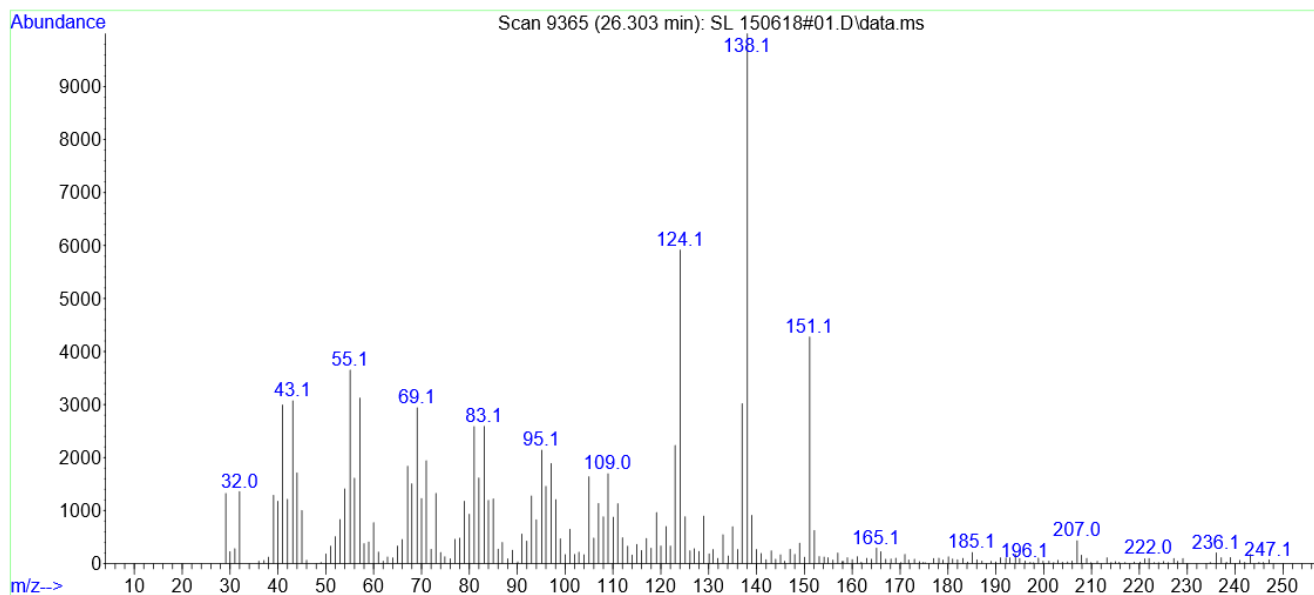
## 102. 2-isopropyl-3-methoxypyrazine



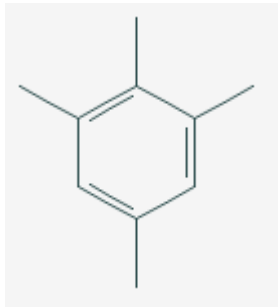
Library Searched : C:\Database\NIST11.L

Quality : 96

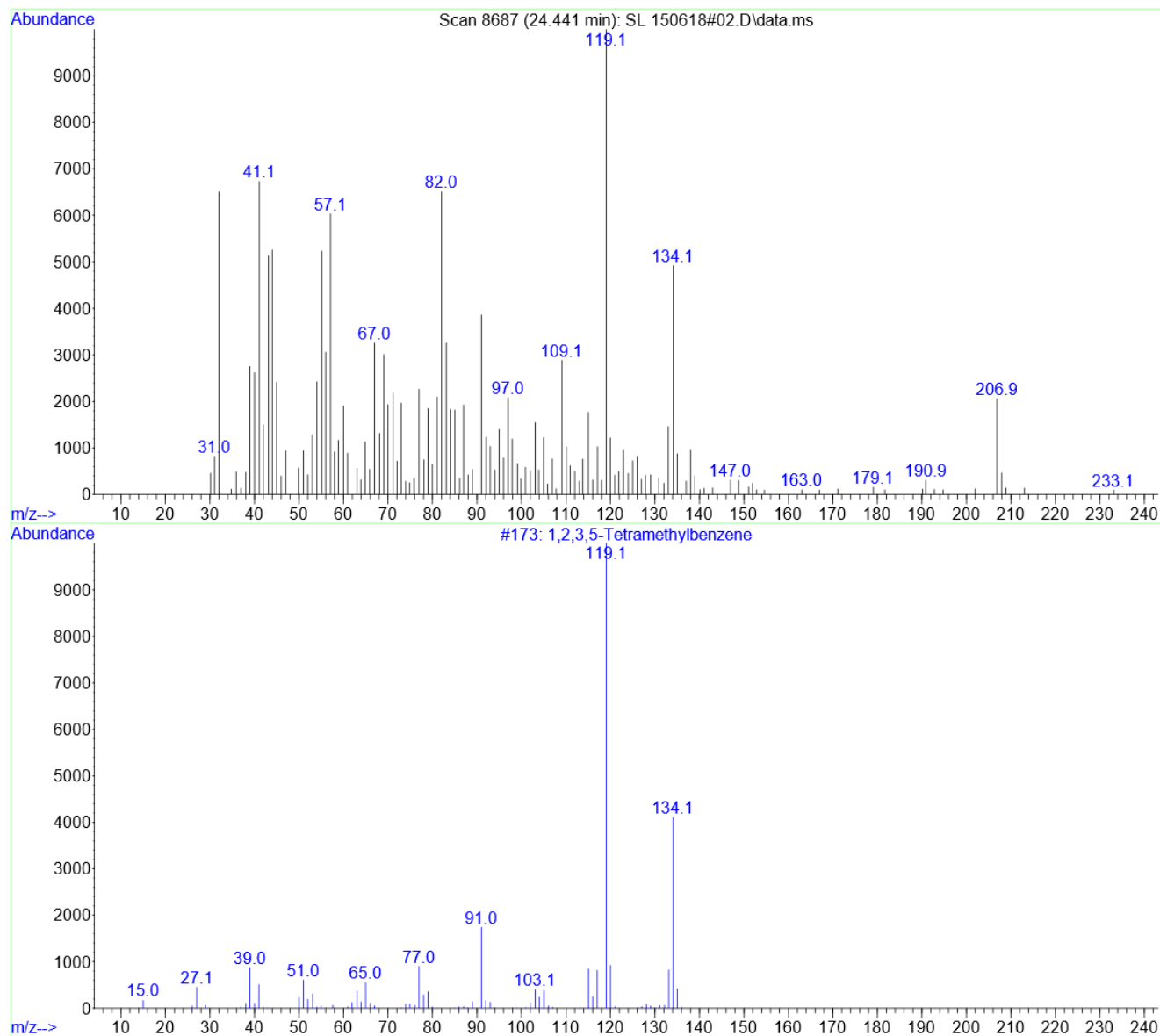
ID : Pyrazine, 2-methoxy-3-(1-methylpropyl)-



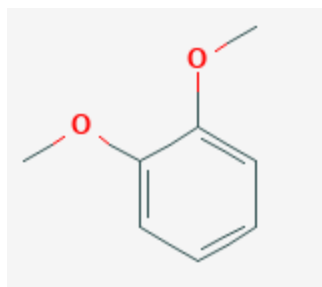
# 103. 1,2,3,5-tetramethylbenzene



Library Searched : C:\Database\LAB429.L  
Quality : 38  
ID : 1,2,3,5-Tetramethylbenzene



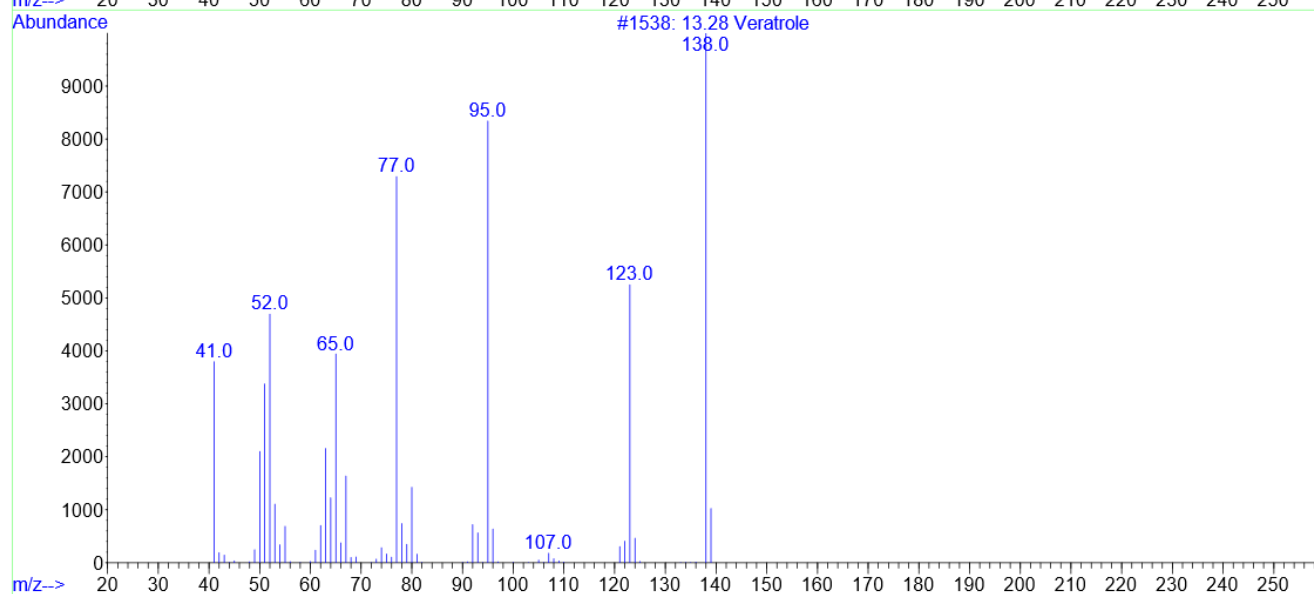
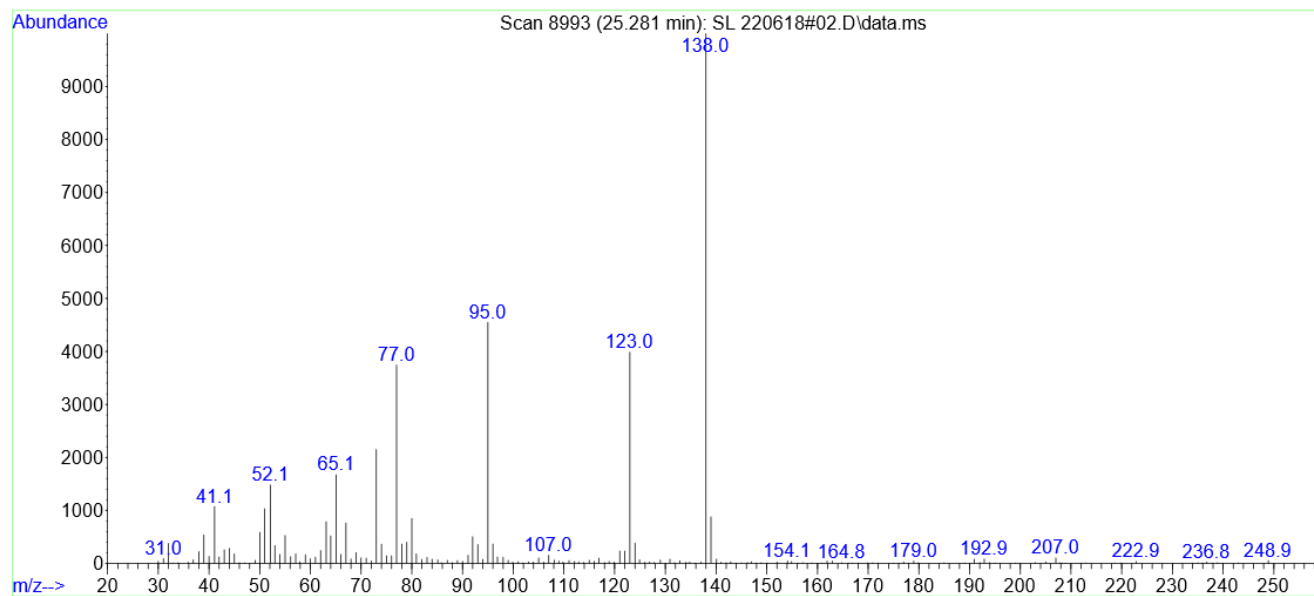
## 104. Veratrole



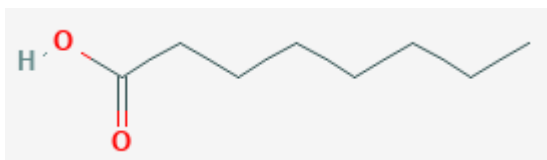
Library Searched : C:\Database\Adams.L

Quality : 87

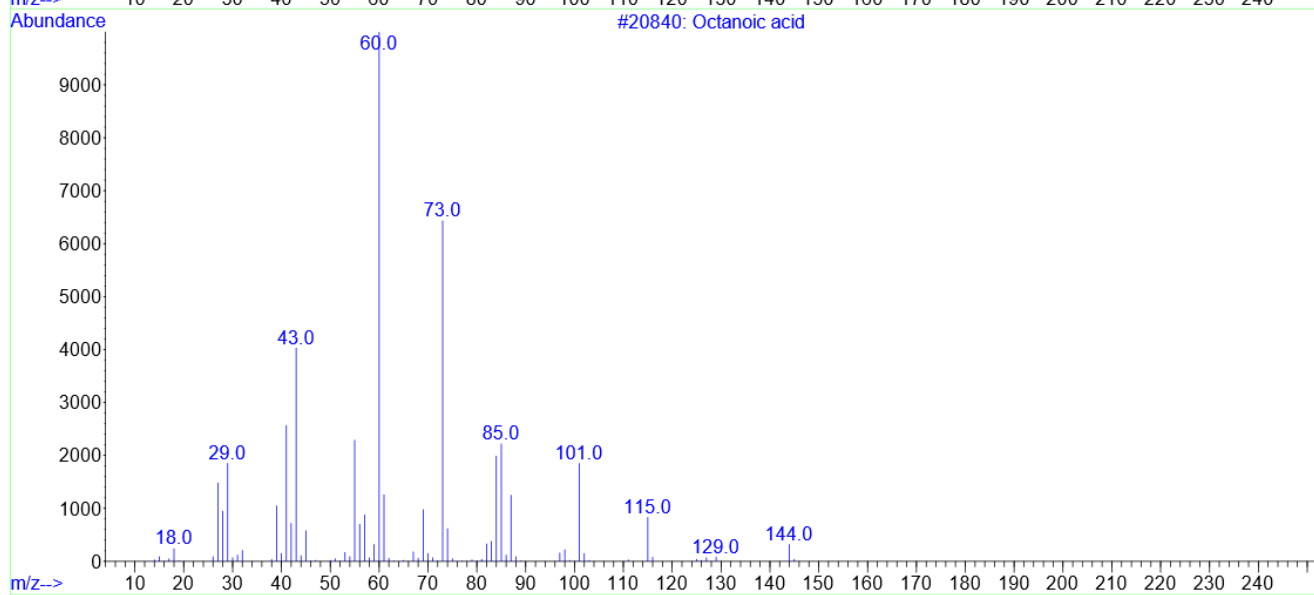
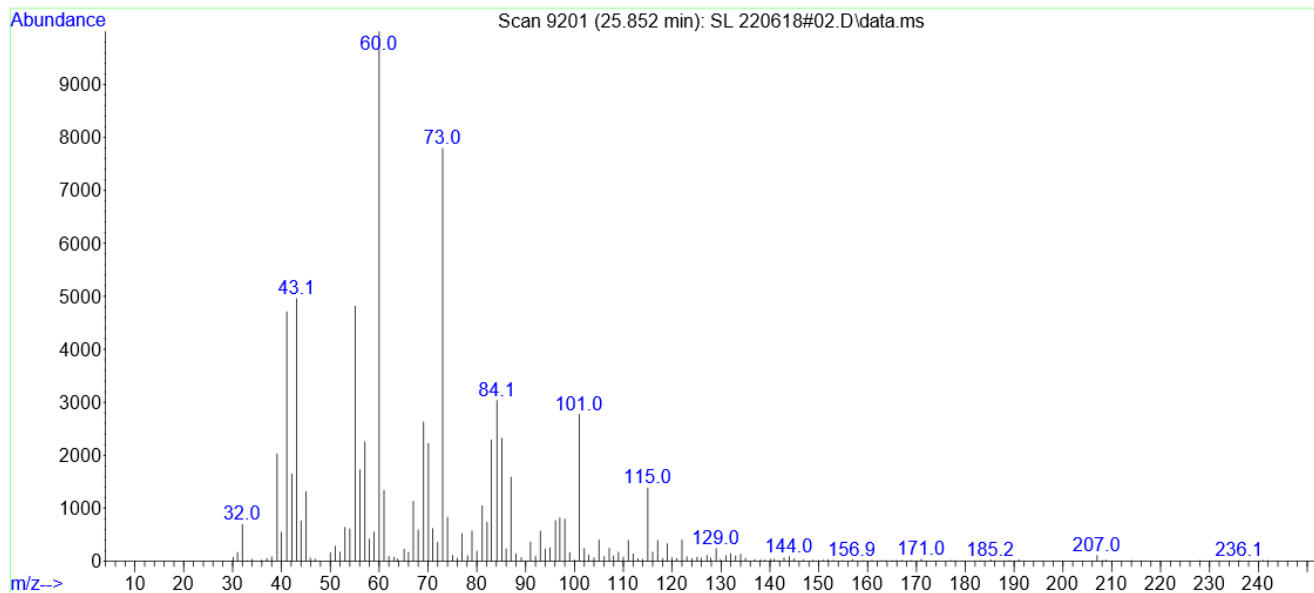
ID : 13.28 Veratrole



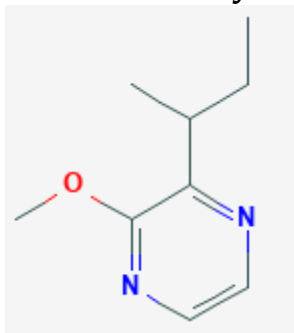
## 105. Octanoic acid



Library Searched : C:\Database\NIST11.L  
Quality : 64  
ID : Octanoic acid



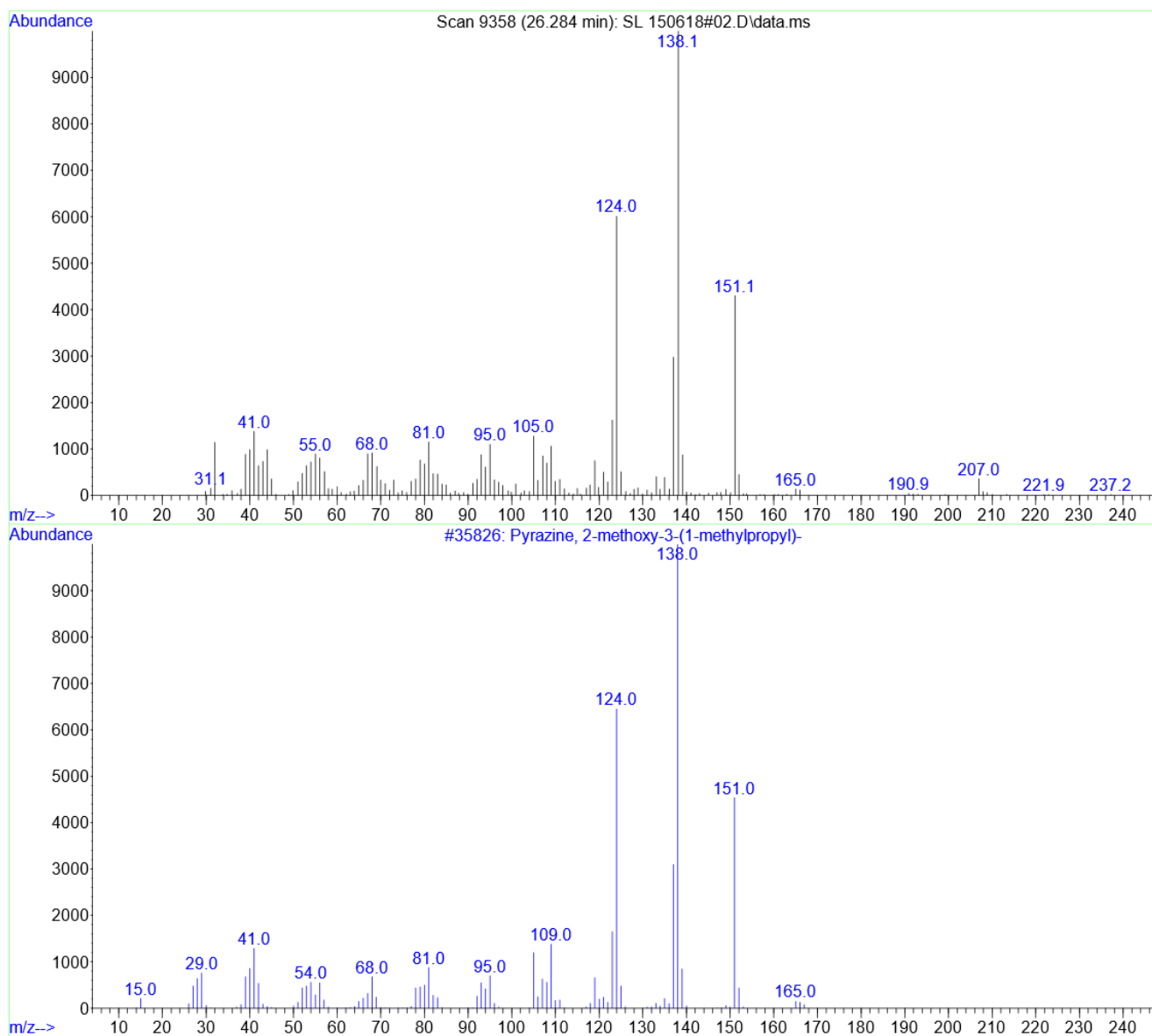
## 106. 2-*sec*-butyl-3-methoxypyrazine



Library Searched : C:\Database\NIST11.L

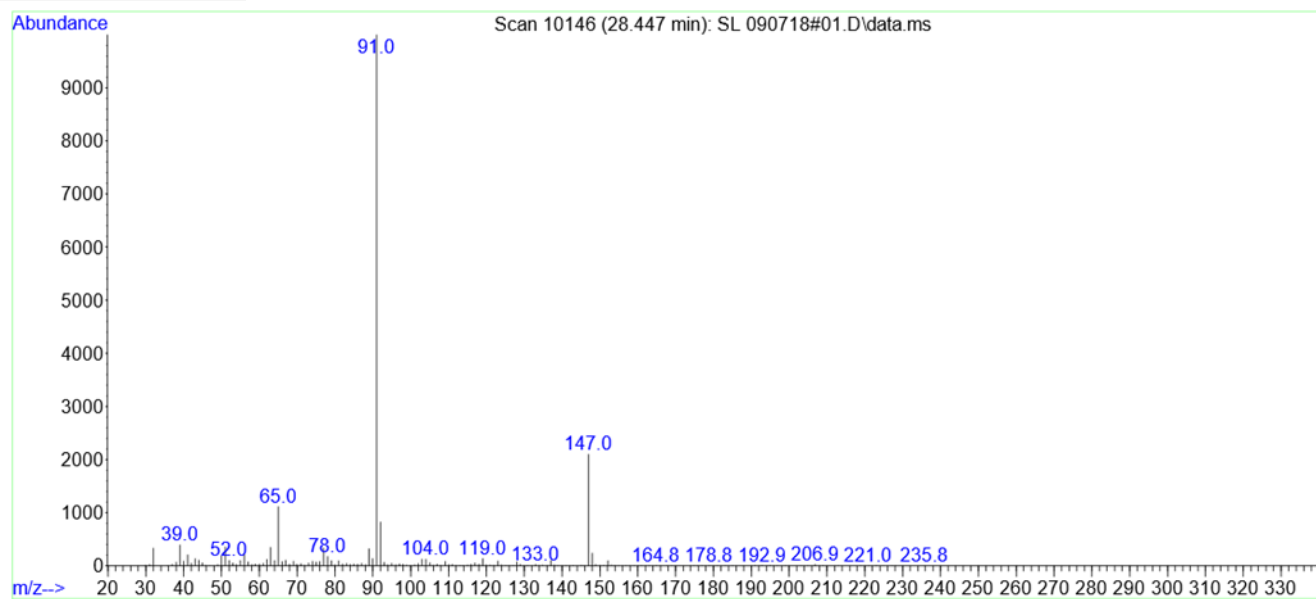
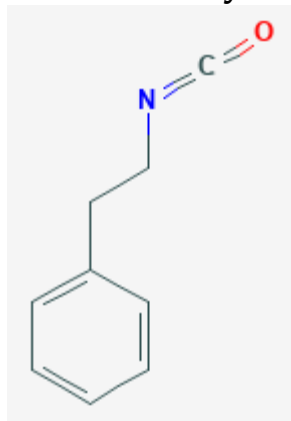
Quality : 97

ID : Pyrazine, 2-methoxy-3-(1-methylpropyl)-

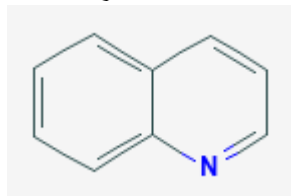




## 107. Phenethyl isocyanate



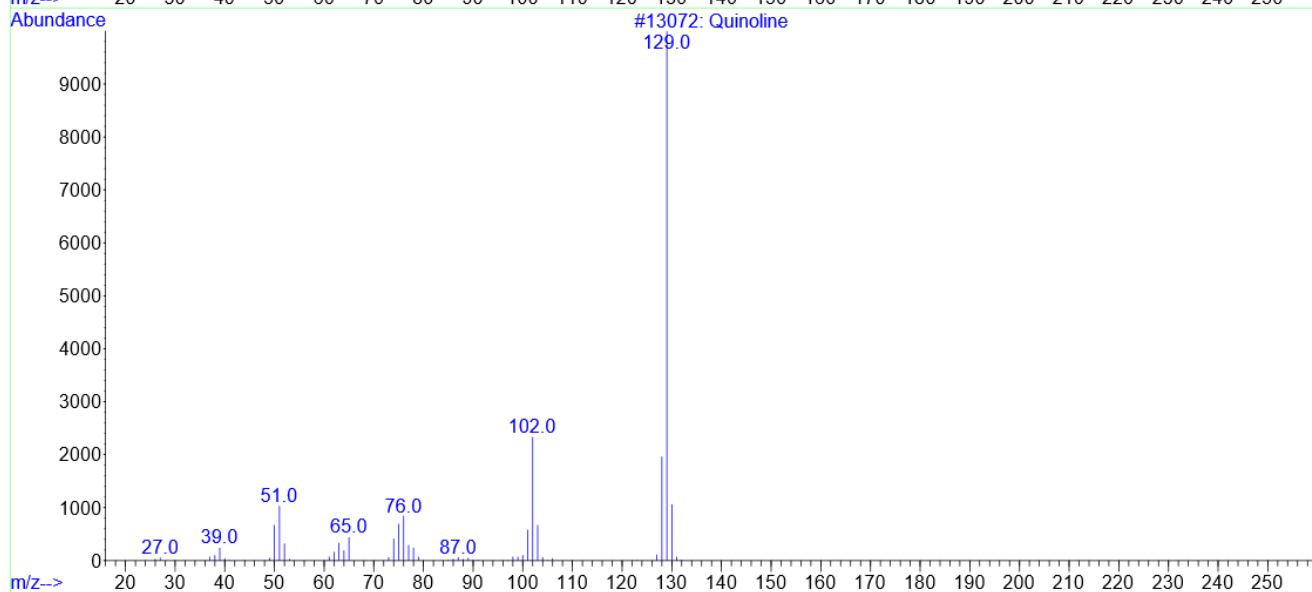
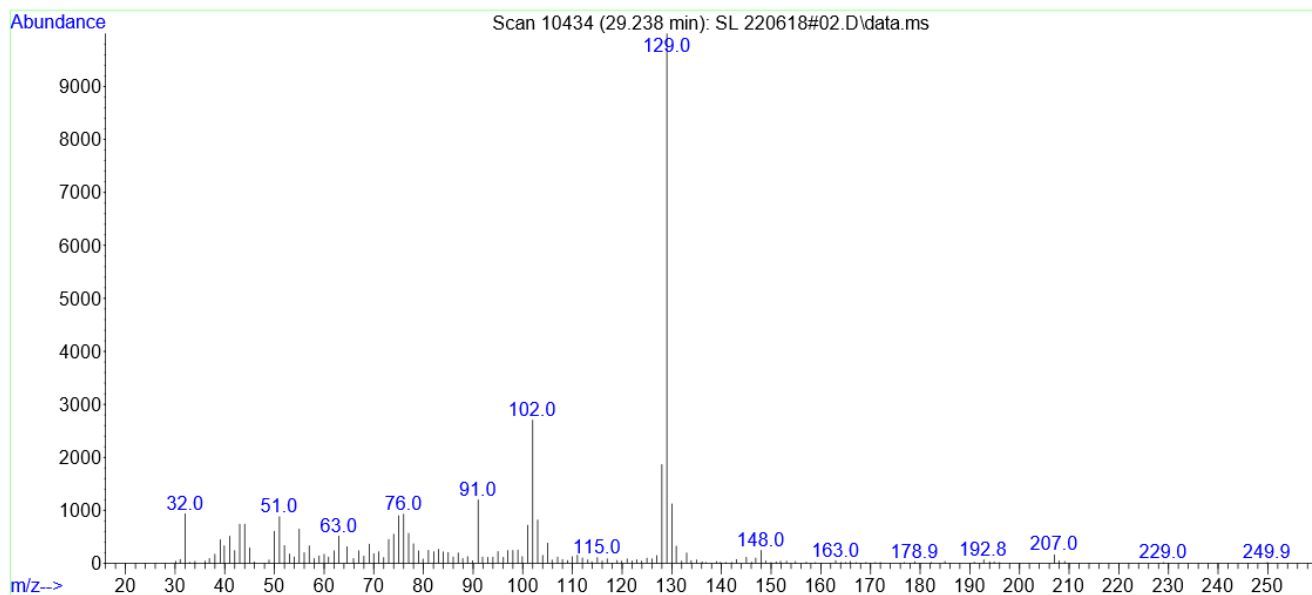
## 108. Quinoline



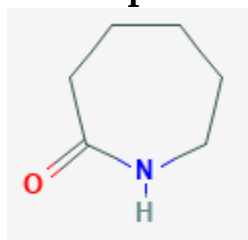
Library Searched : C:\Database\NIST11.L

Quality : 95

ID : Quinoline



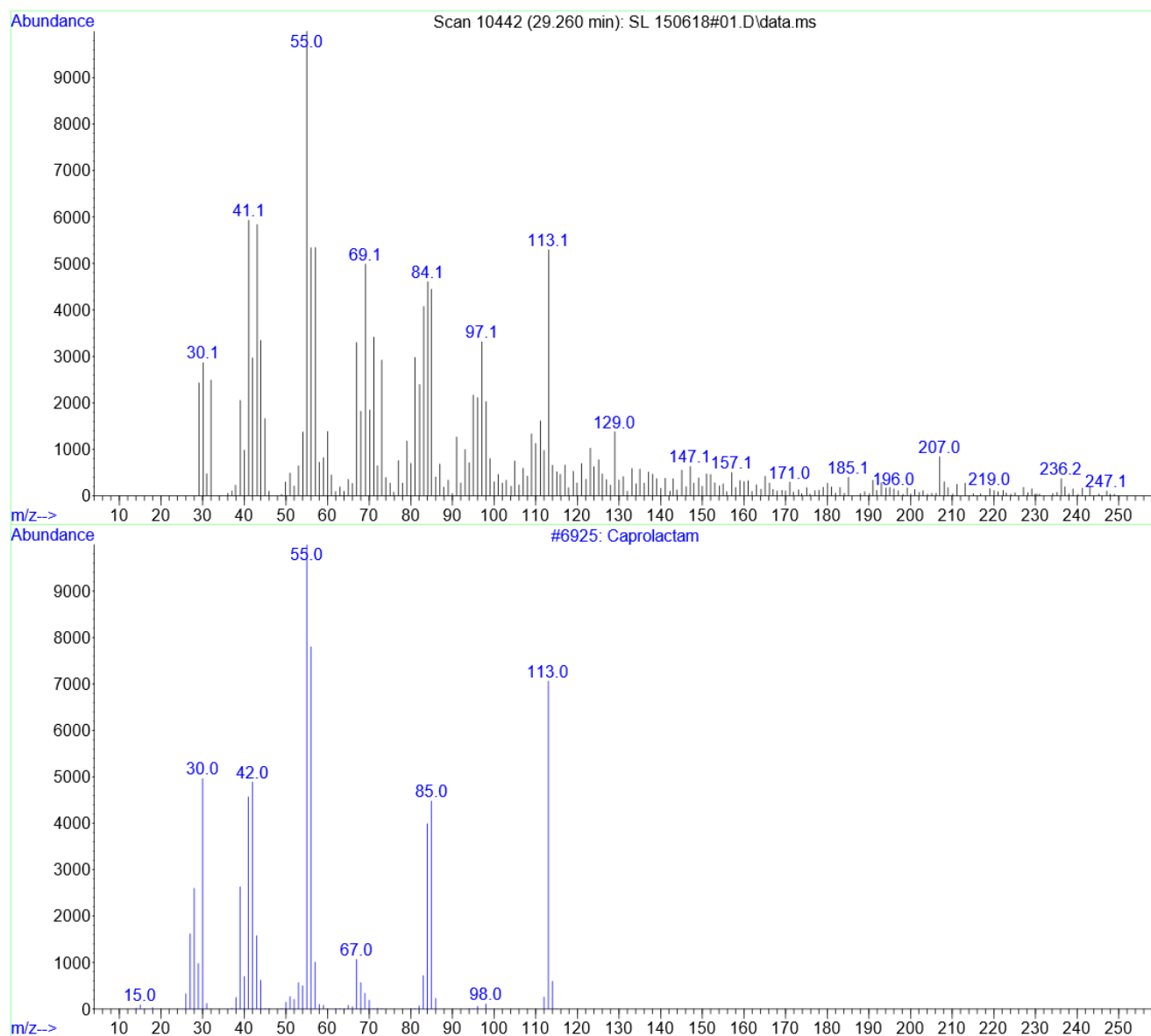
## 109. Caprolactam



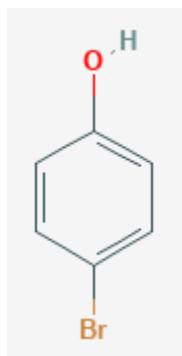
Library Searched : C:\Database\NIST11.L

Quality : 46

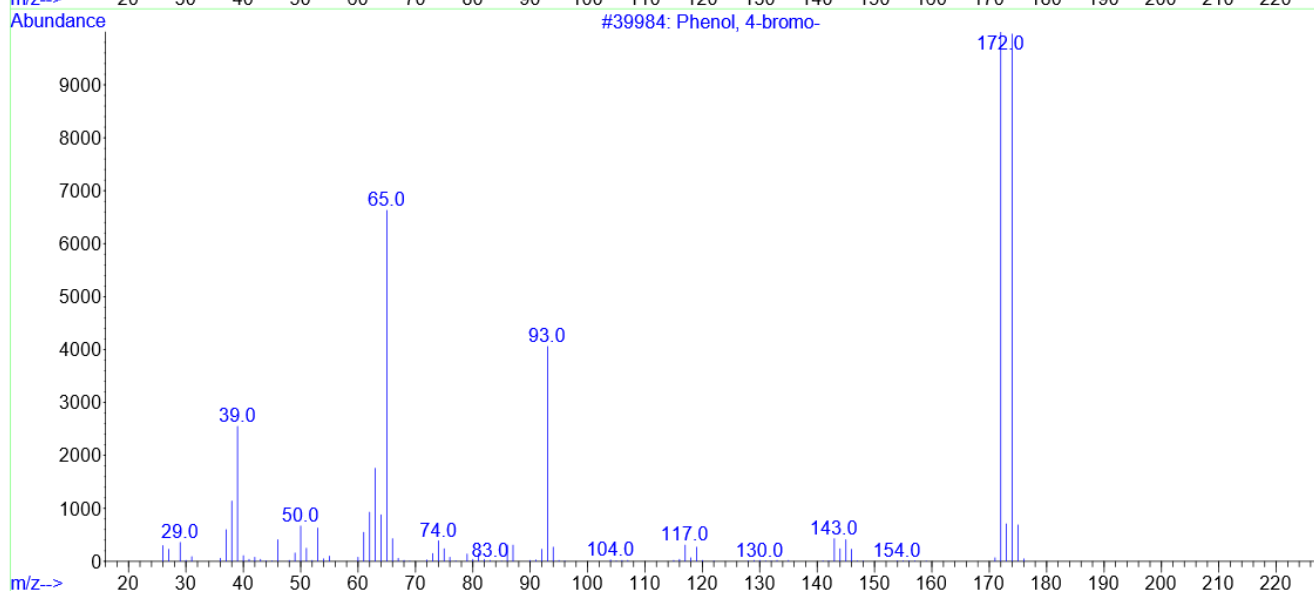
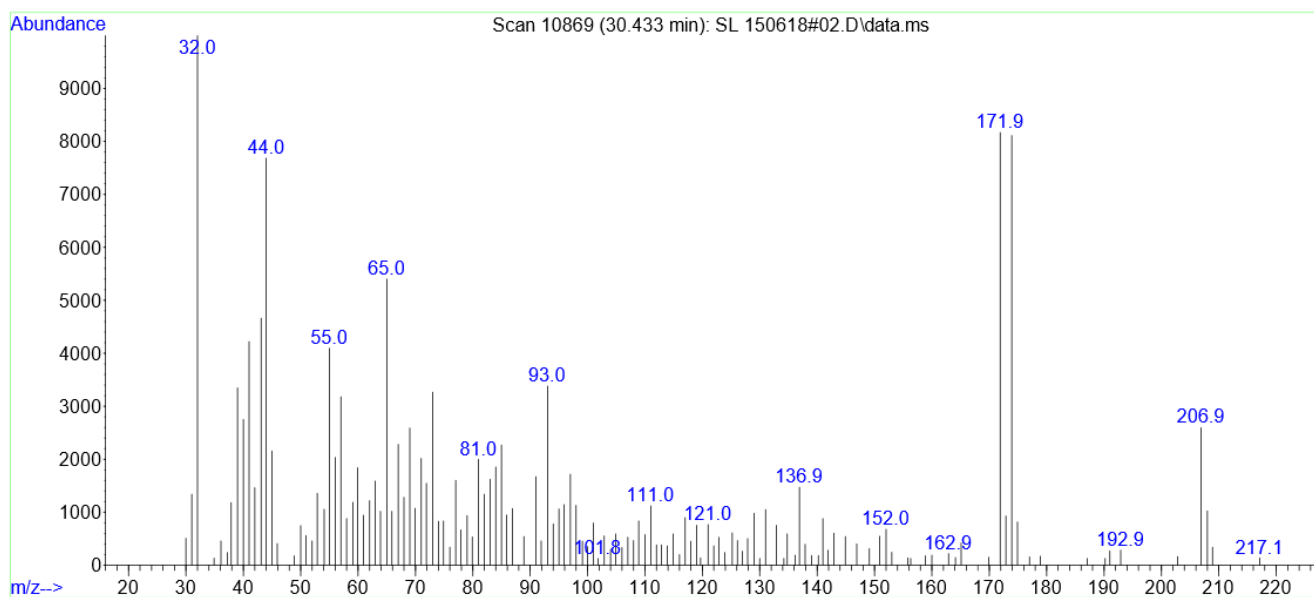
ID : Caprolactam



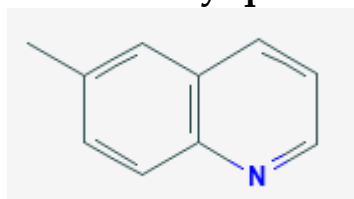
# 110. 4-bromophenol



Library Searched : C:\Database\NIST11.L  
Quality : 97  
ID : Phenol, 4-bromo-



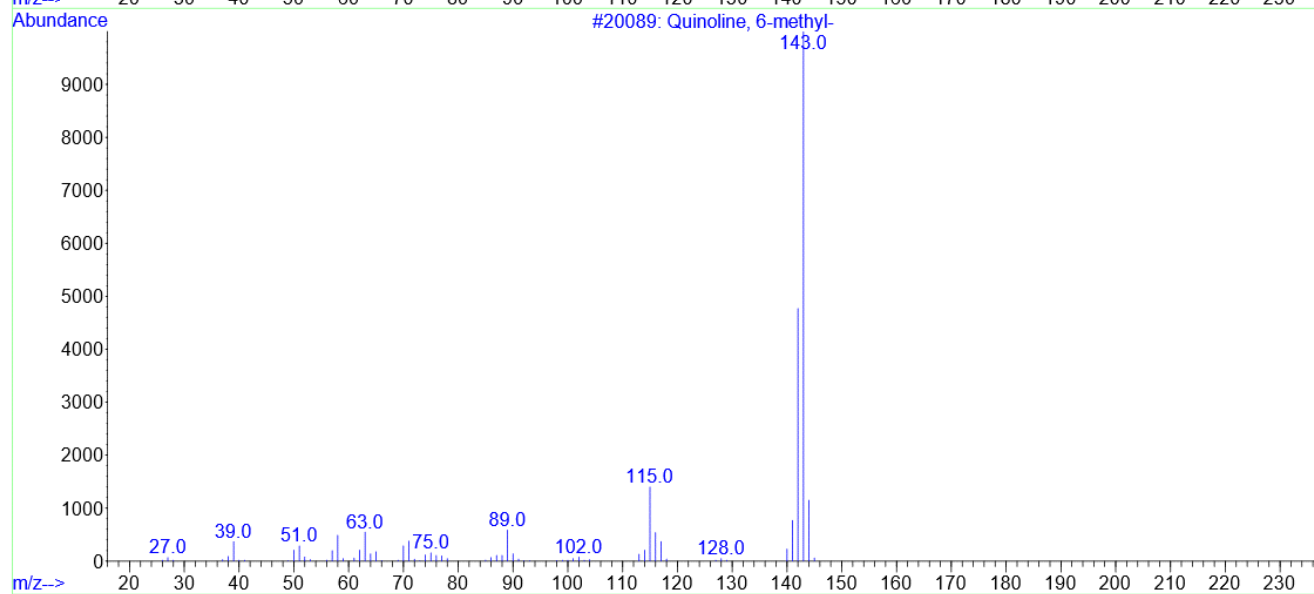
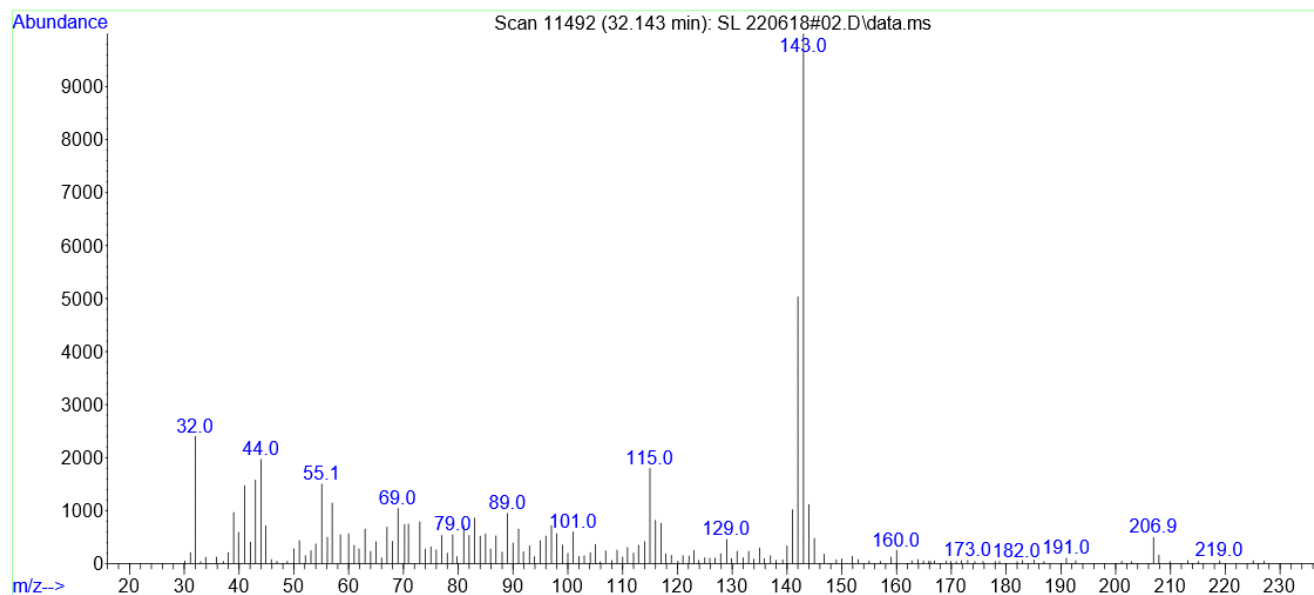
# 111. 6-methylquinoline



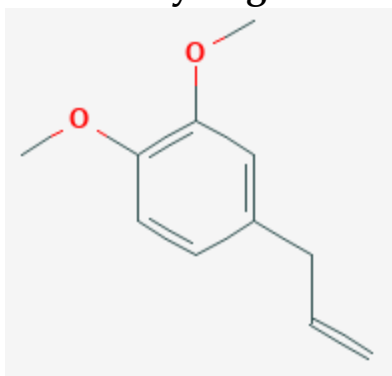
Library Searched : C:\Database\NIST11.L

Quality : 94

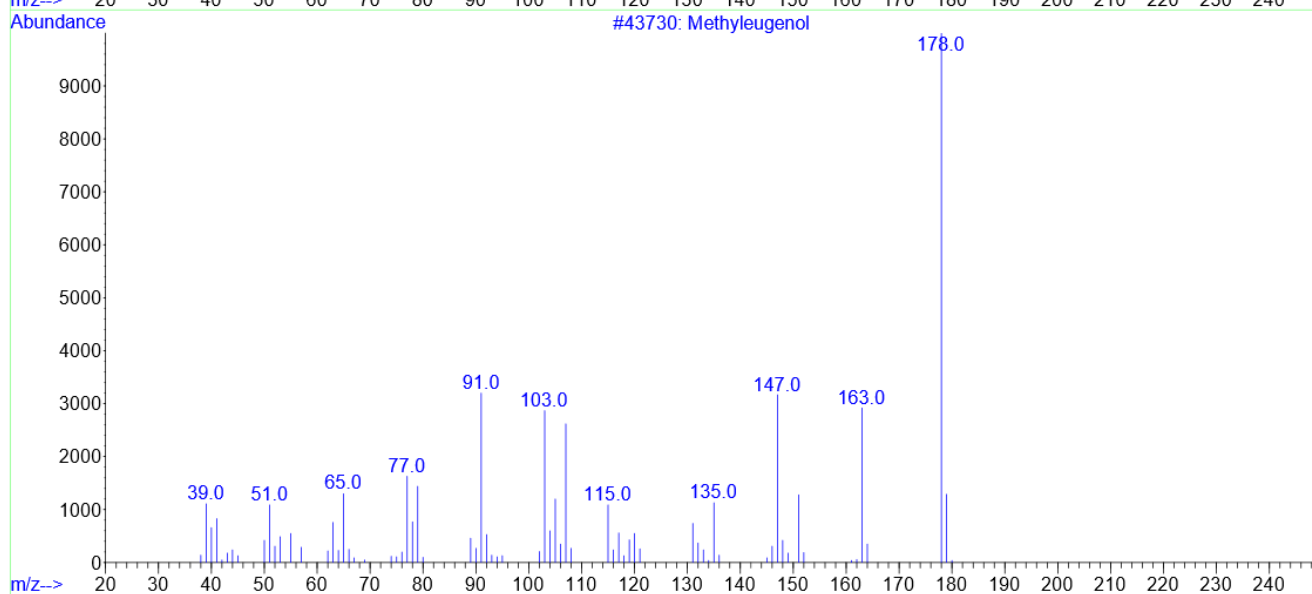
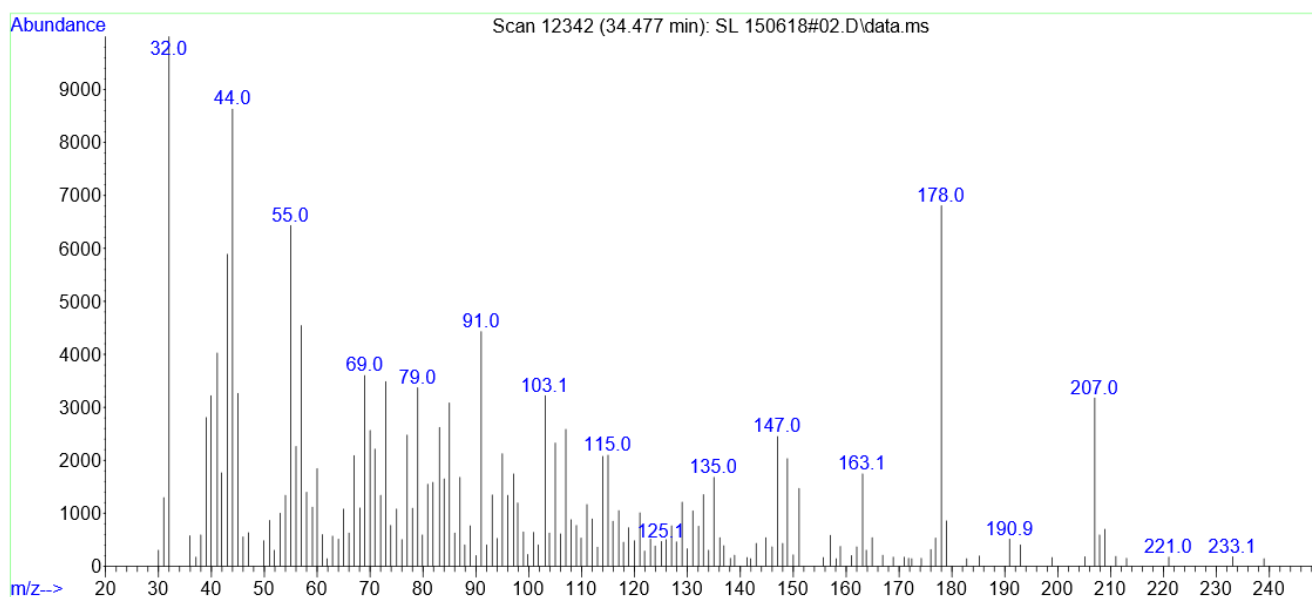
ID : Quinoline, 6-methyl-



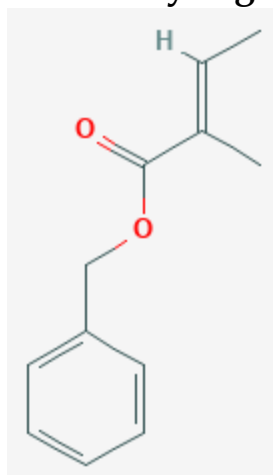
## 112. Methyleugenol



Library Searched : C:\Database\NIST11.L  
Quality : 64  
ID : Methyleugenol



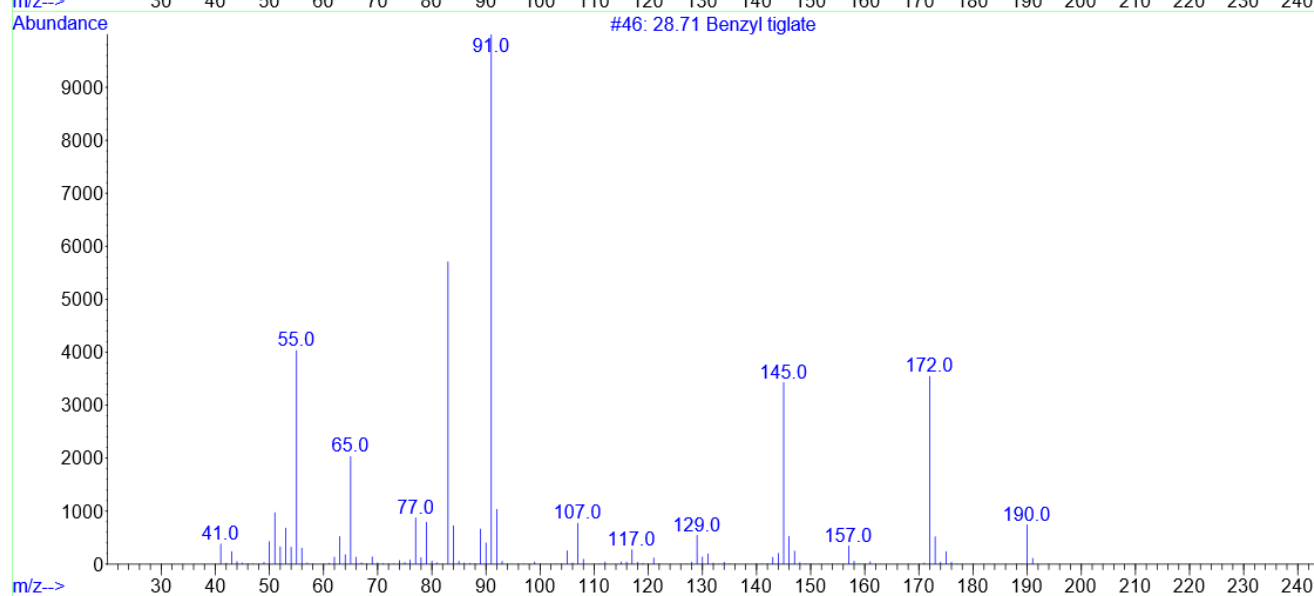
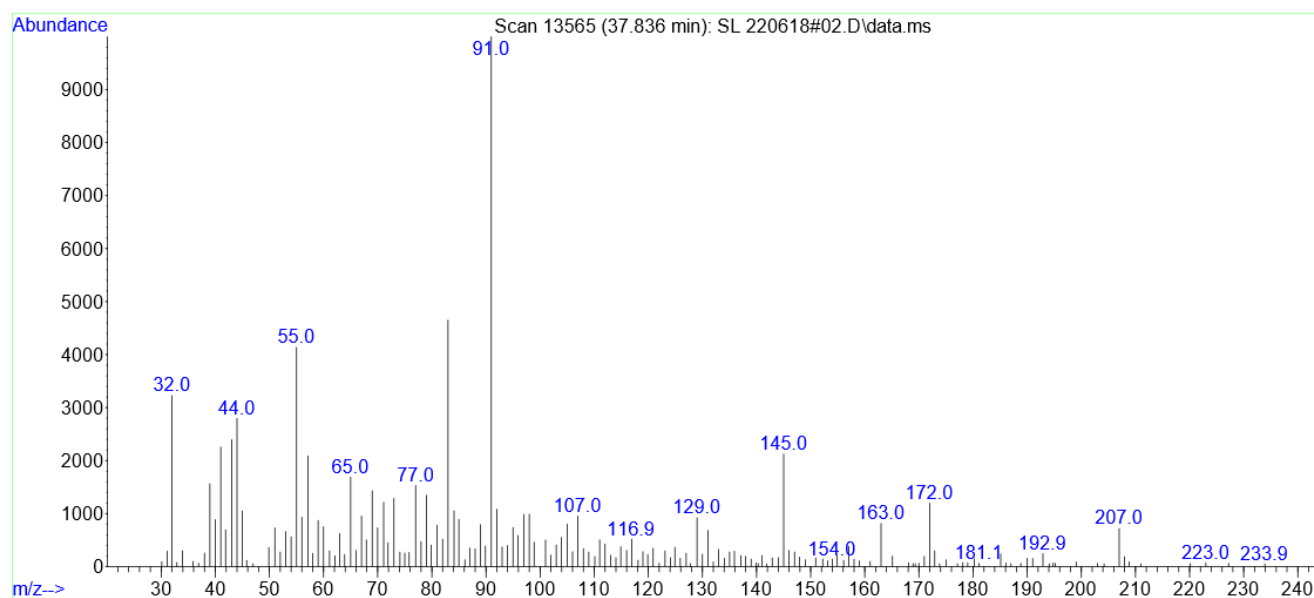
## 113. Benzyl tiglate



Library Searched : C:\Database\Adams.L

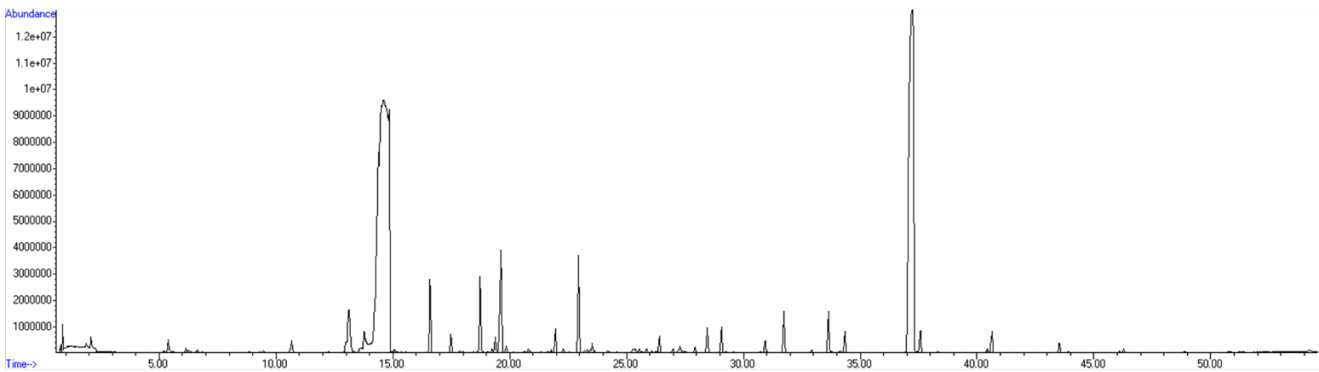
Quality : 64

ID : 28.71 Benzyl tiglate

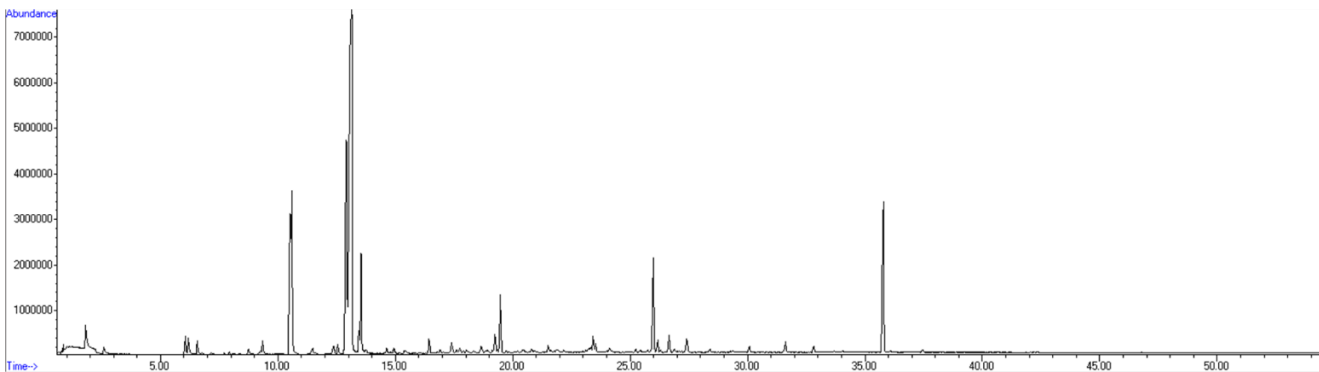


# GC-MS chromatograms

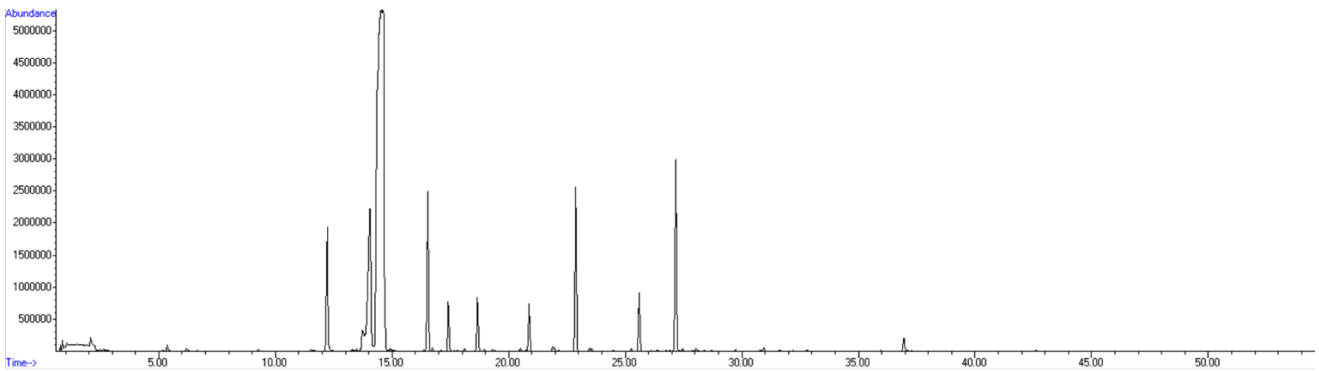
Horseradish



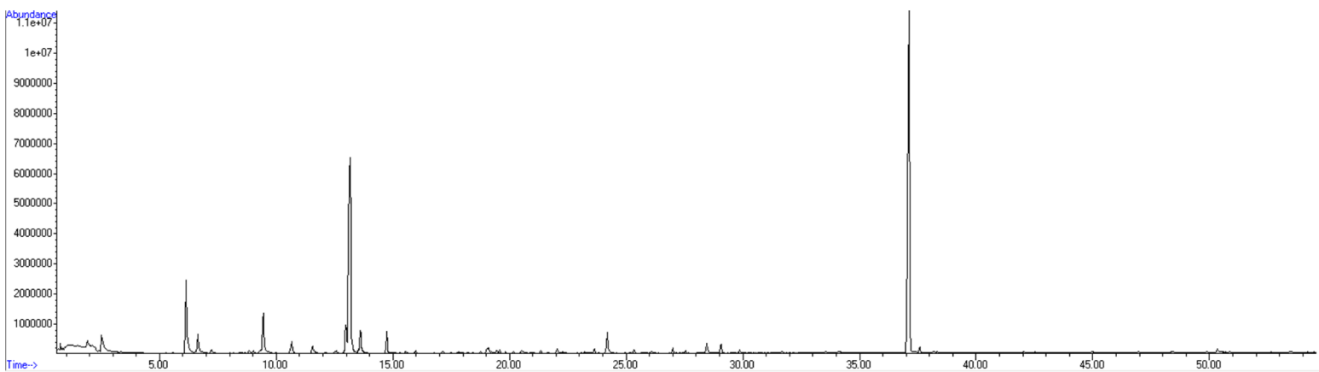
Rocket



Wasabi



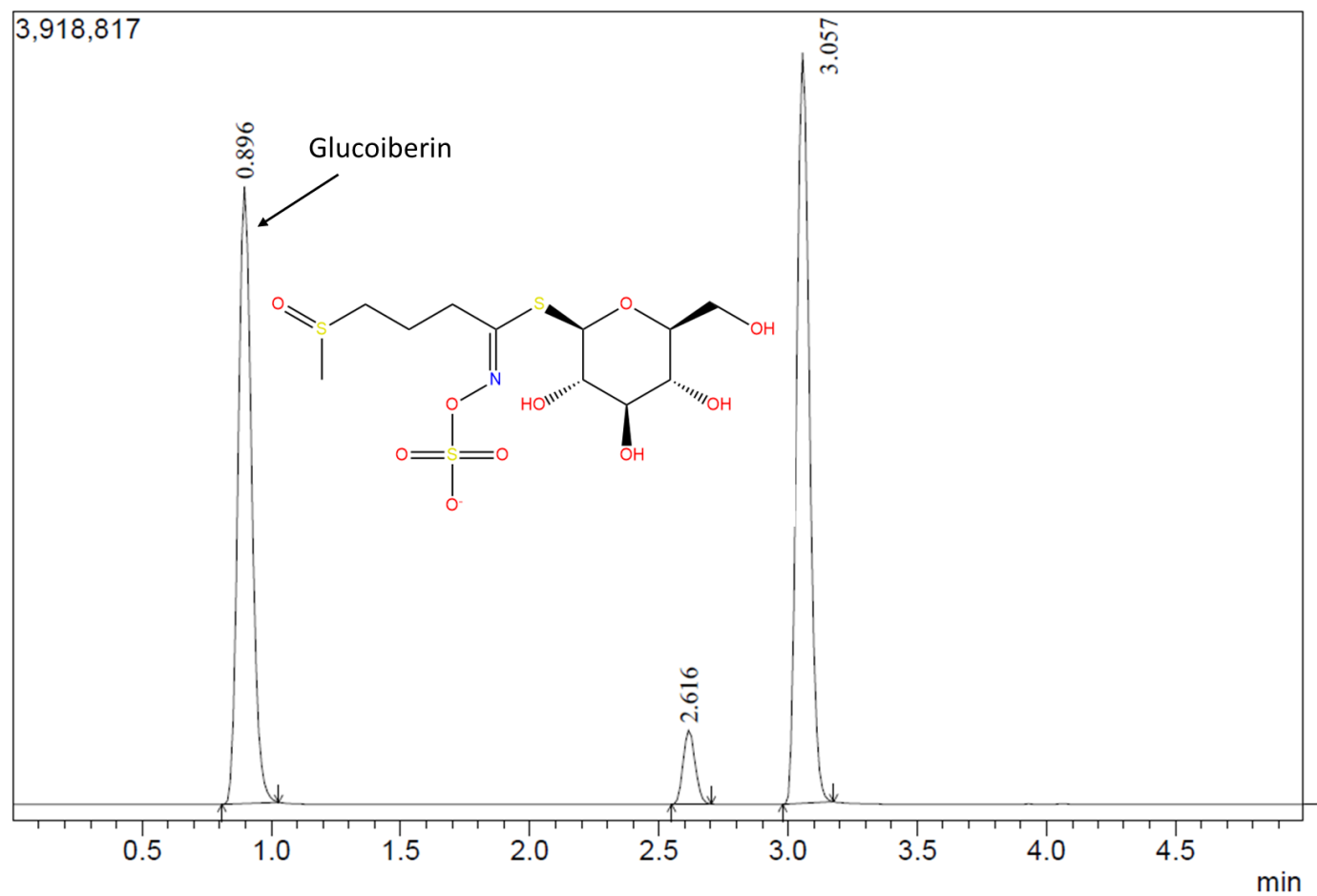
Watercress



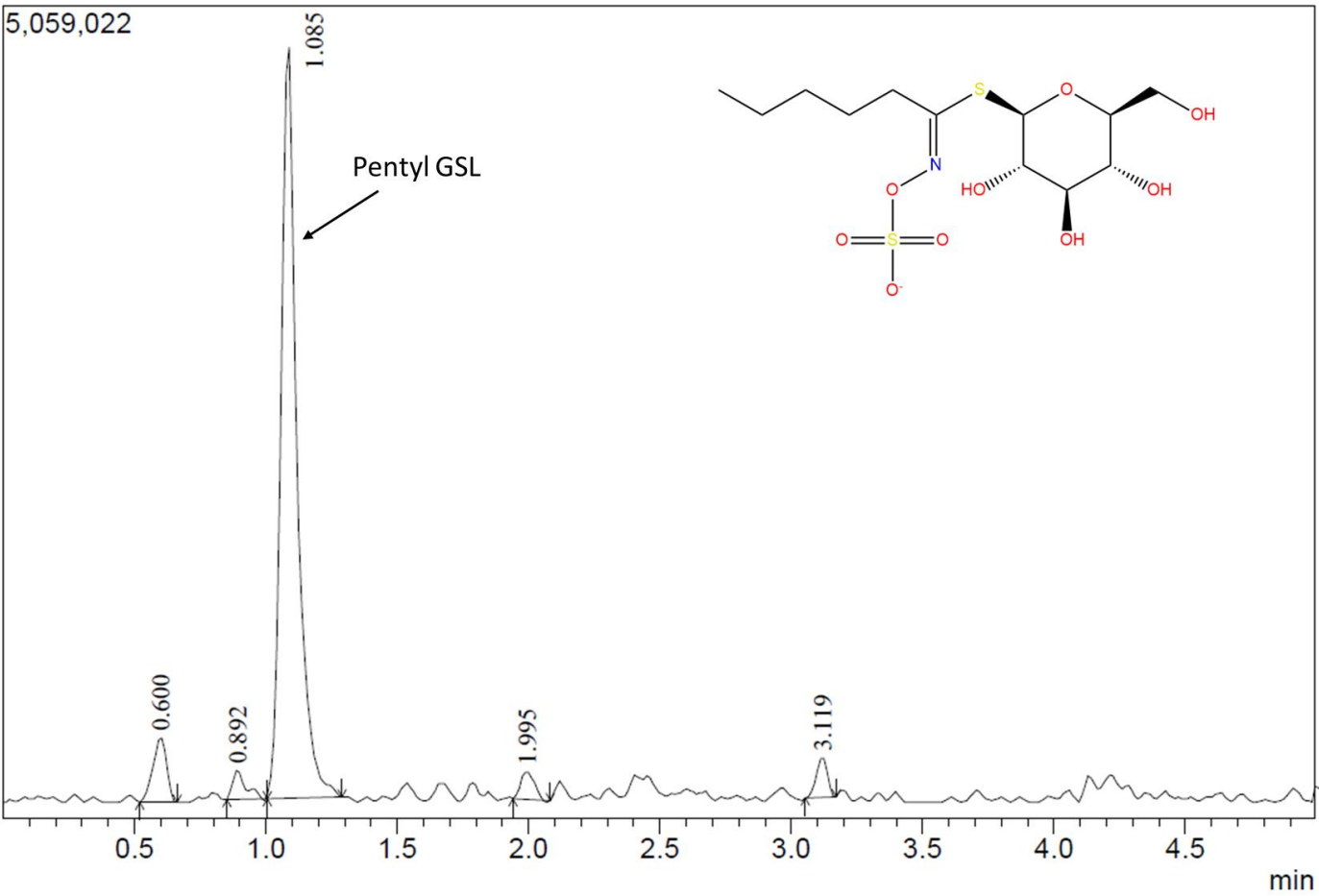


**Supplementary data S2. Total Ion Chromatograms (TICs) of glucosinolates identified by UPLC-MS/MS.**

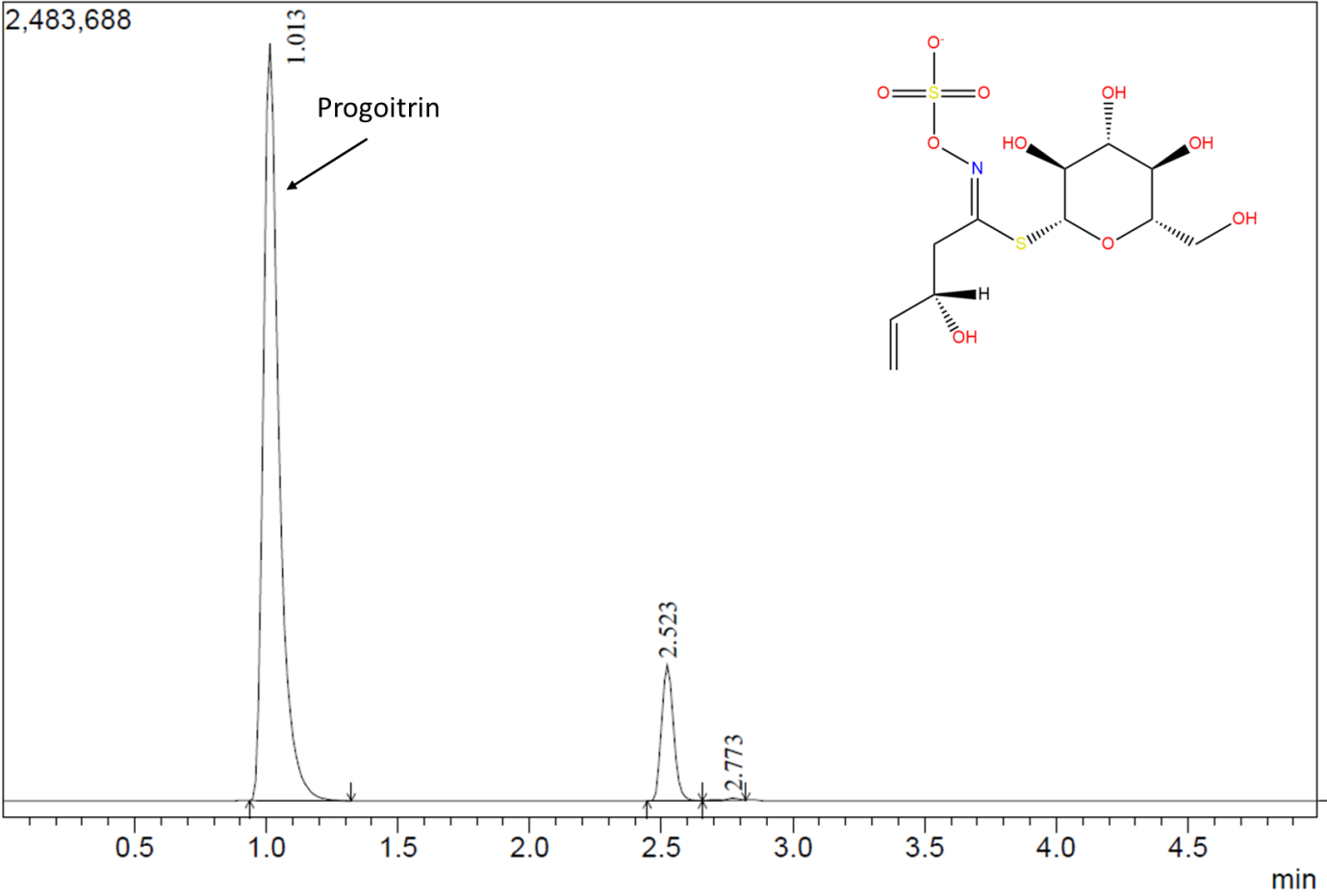
**Glucoiberin**



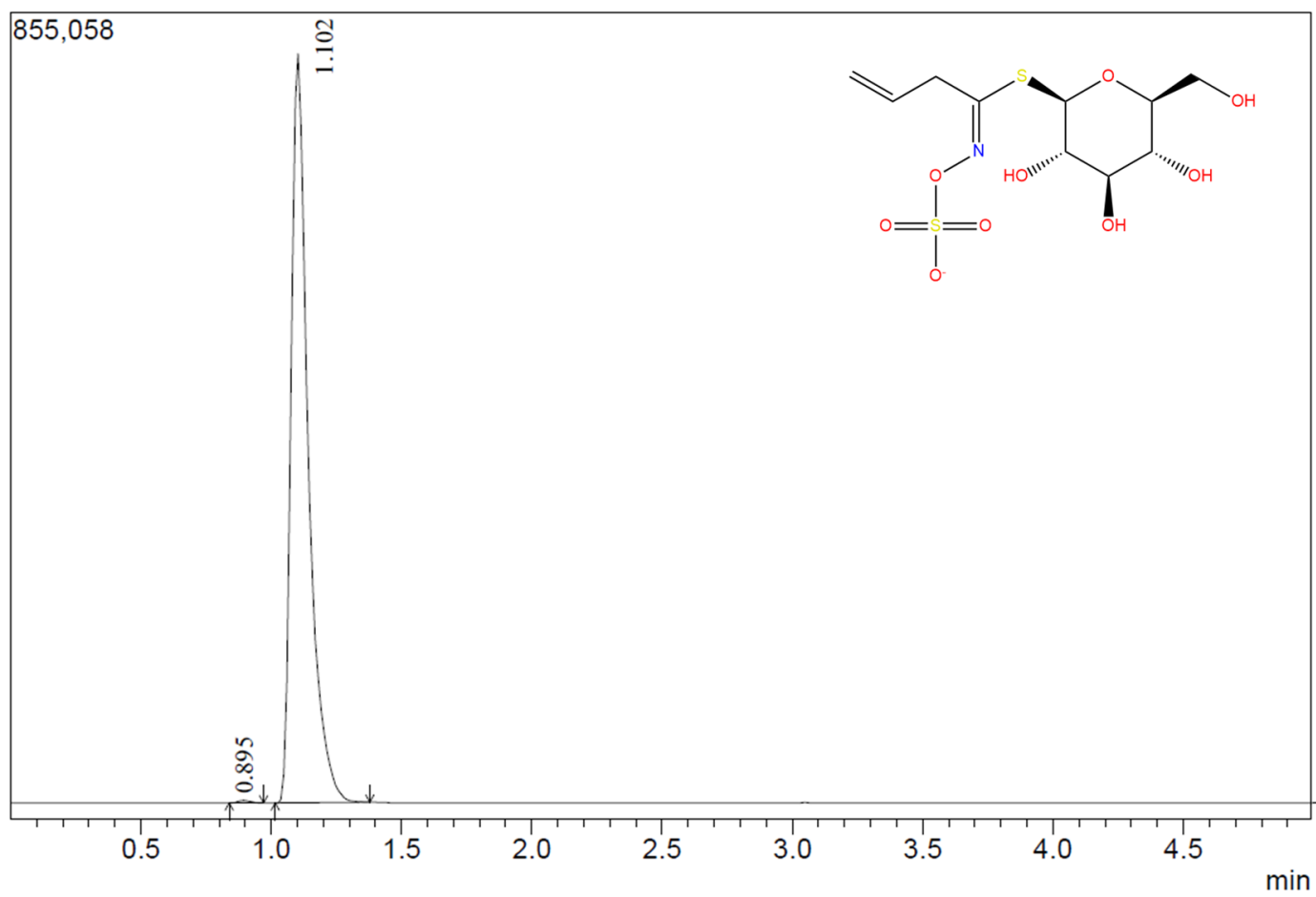
Pentyl GSL



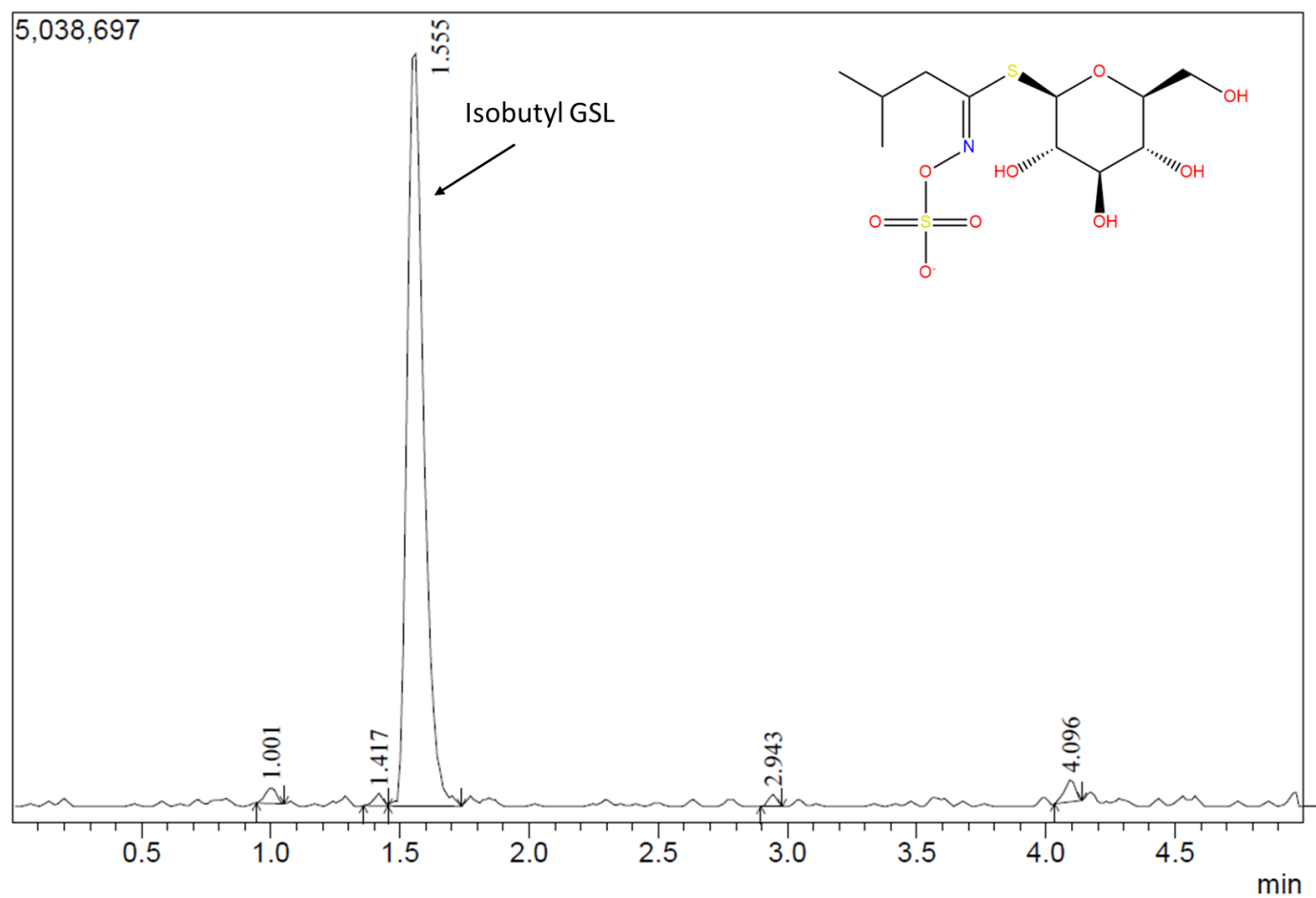
Progoitrin



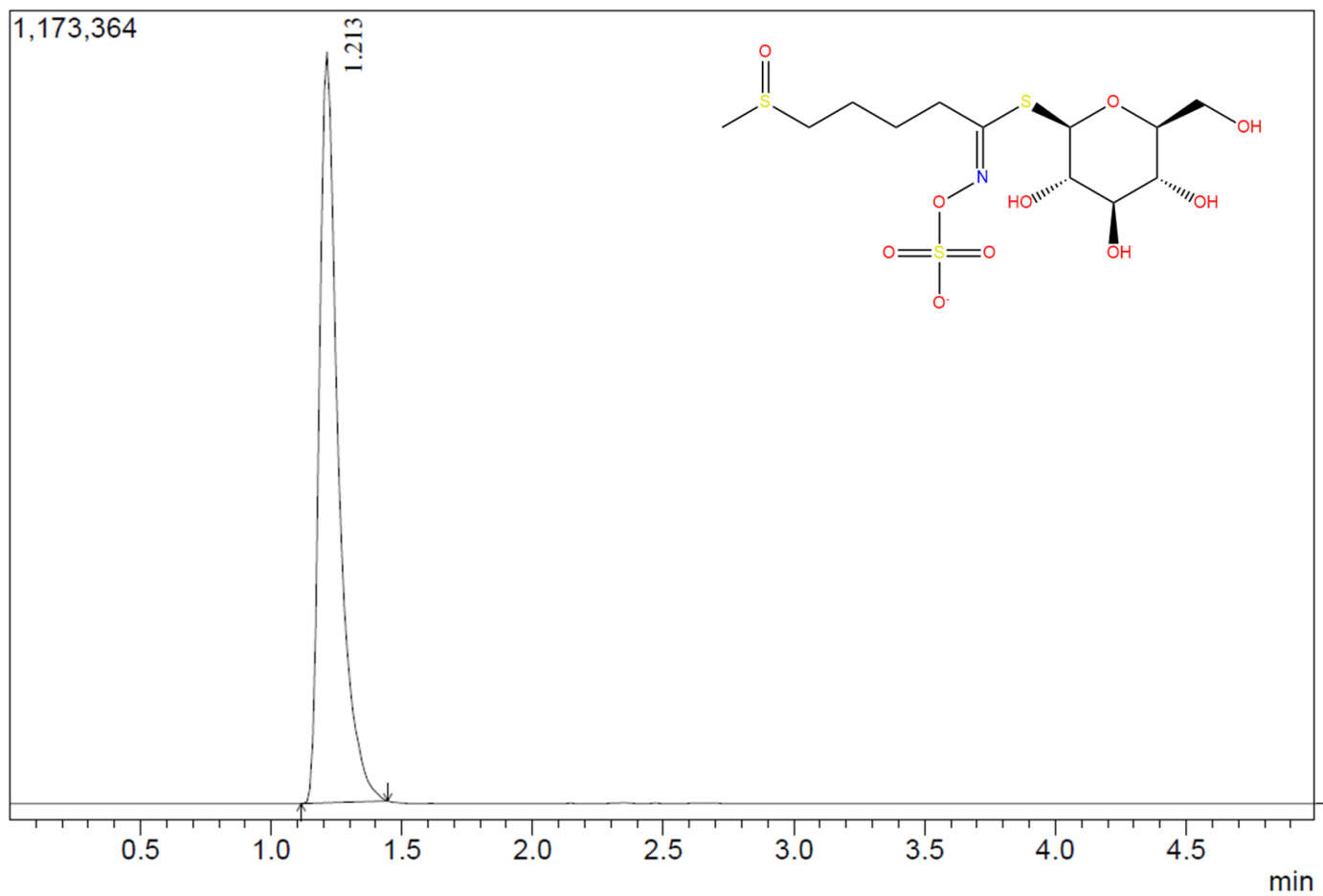
# Sinigrin



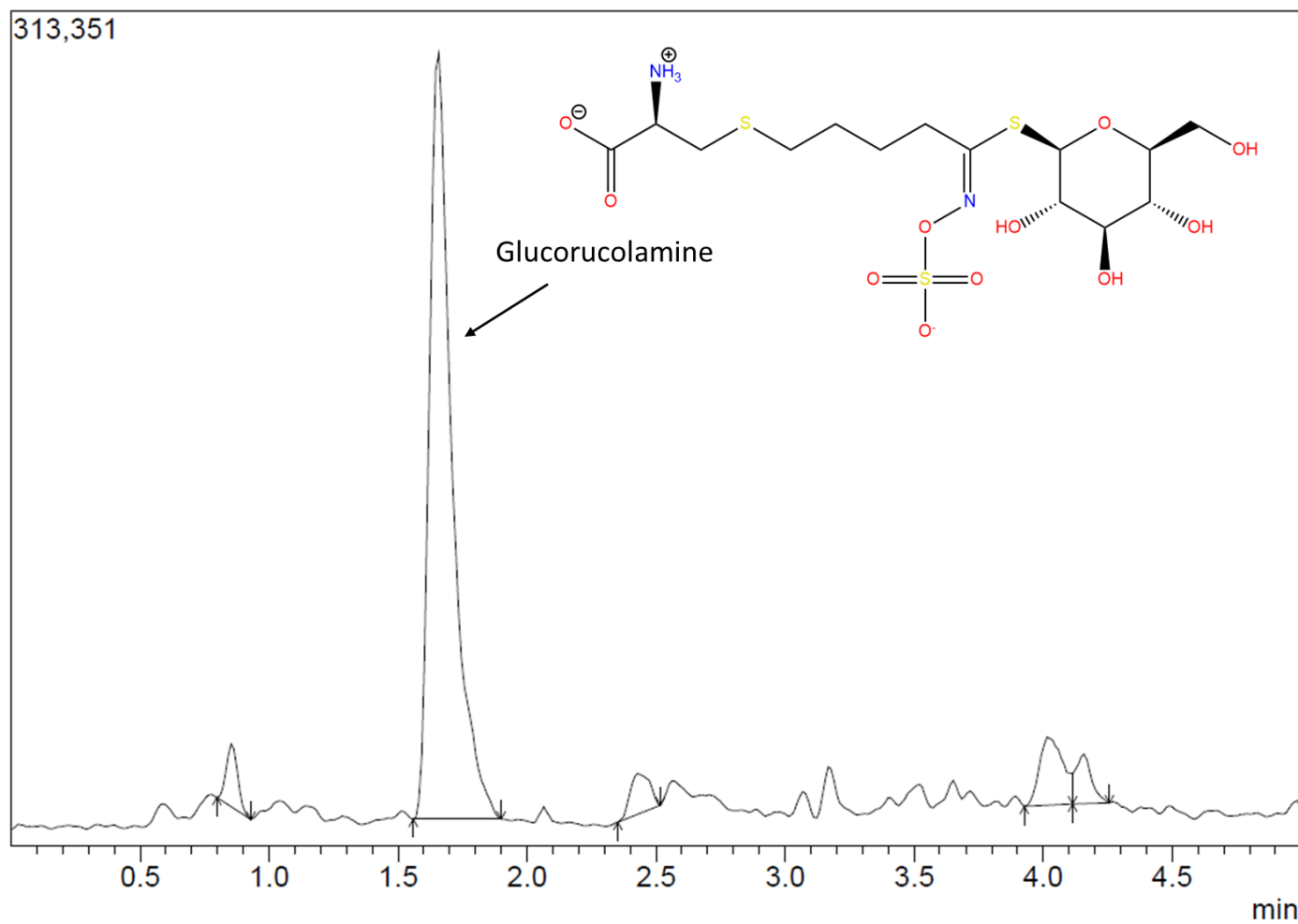
# Isobutyl GSL



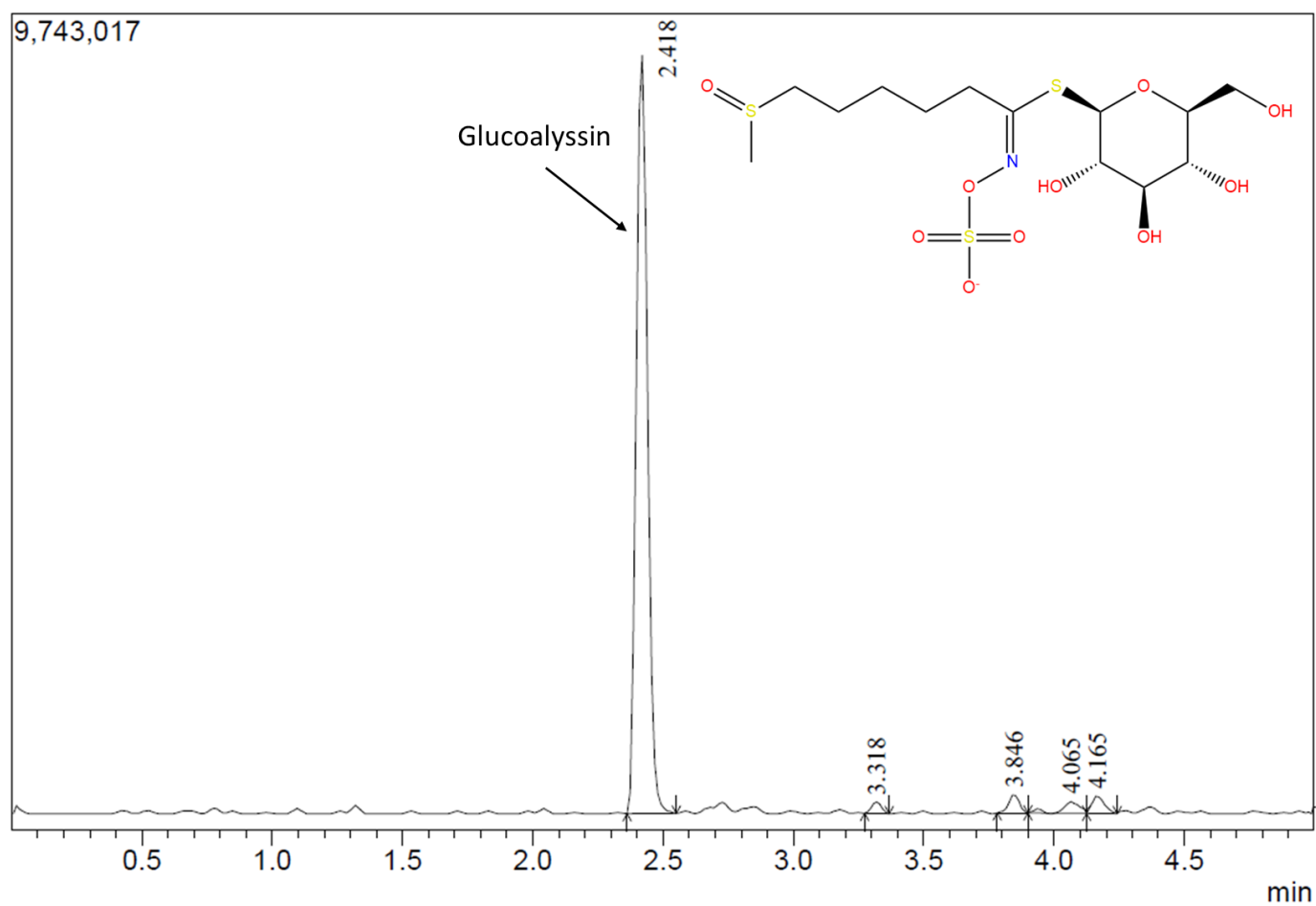
# Glucoraphanin



# Glucorucolamine

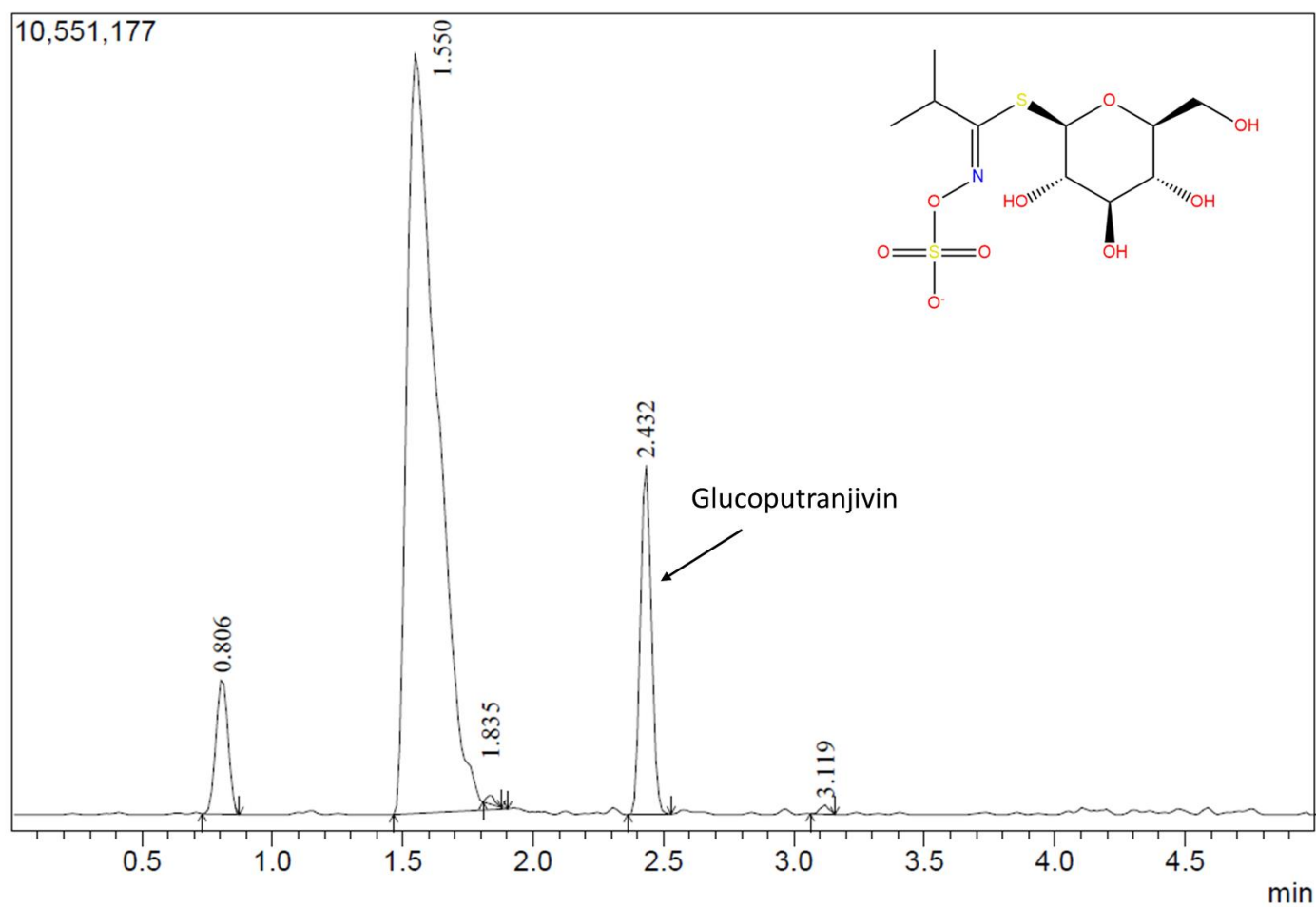


# Glucoalyssin

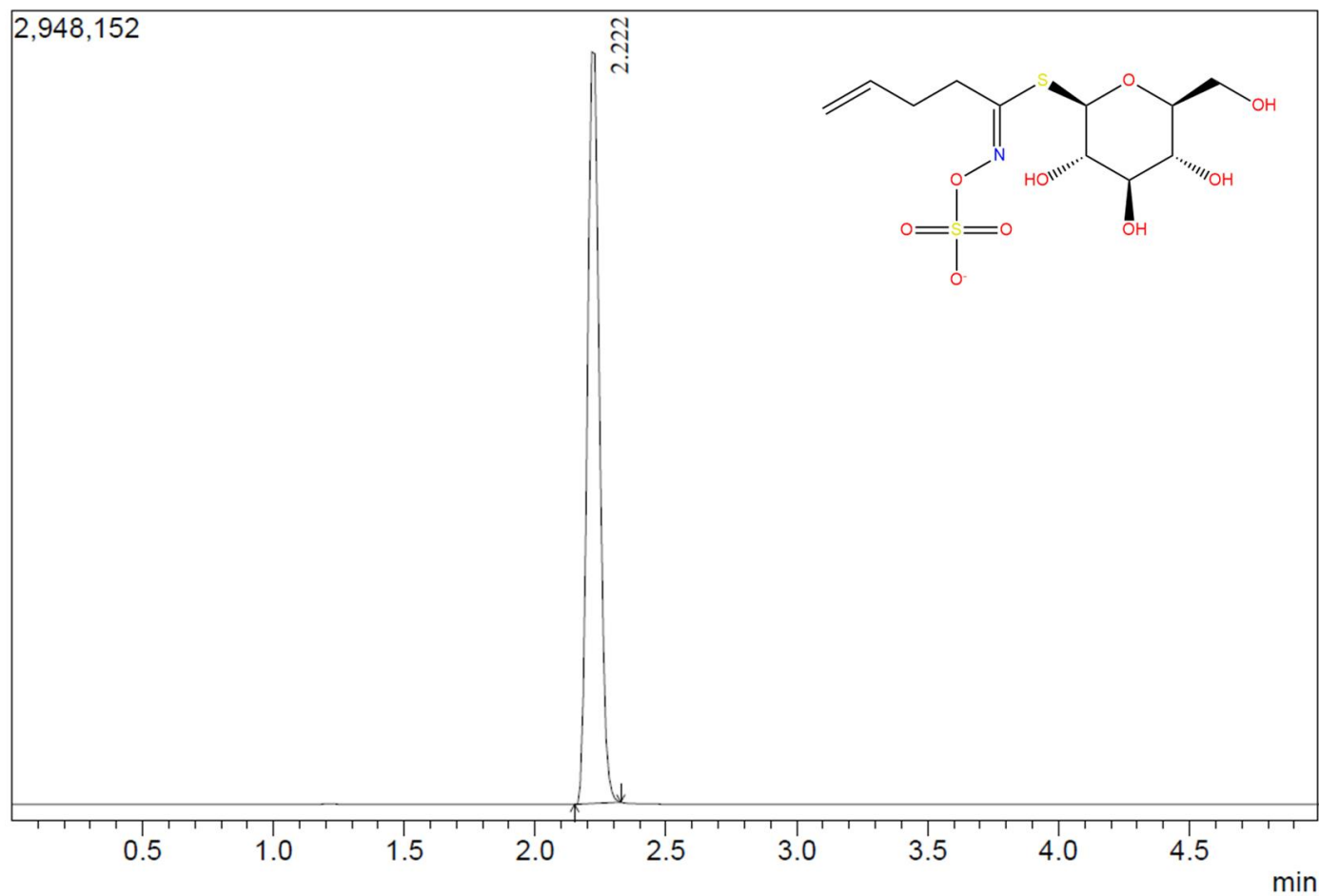




# Glucoputranjivin

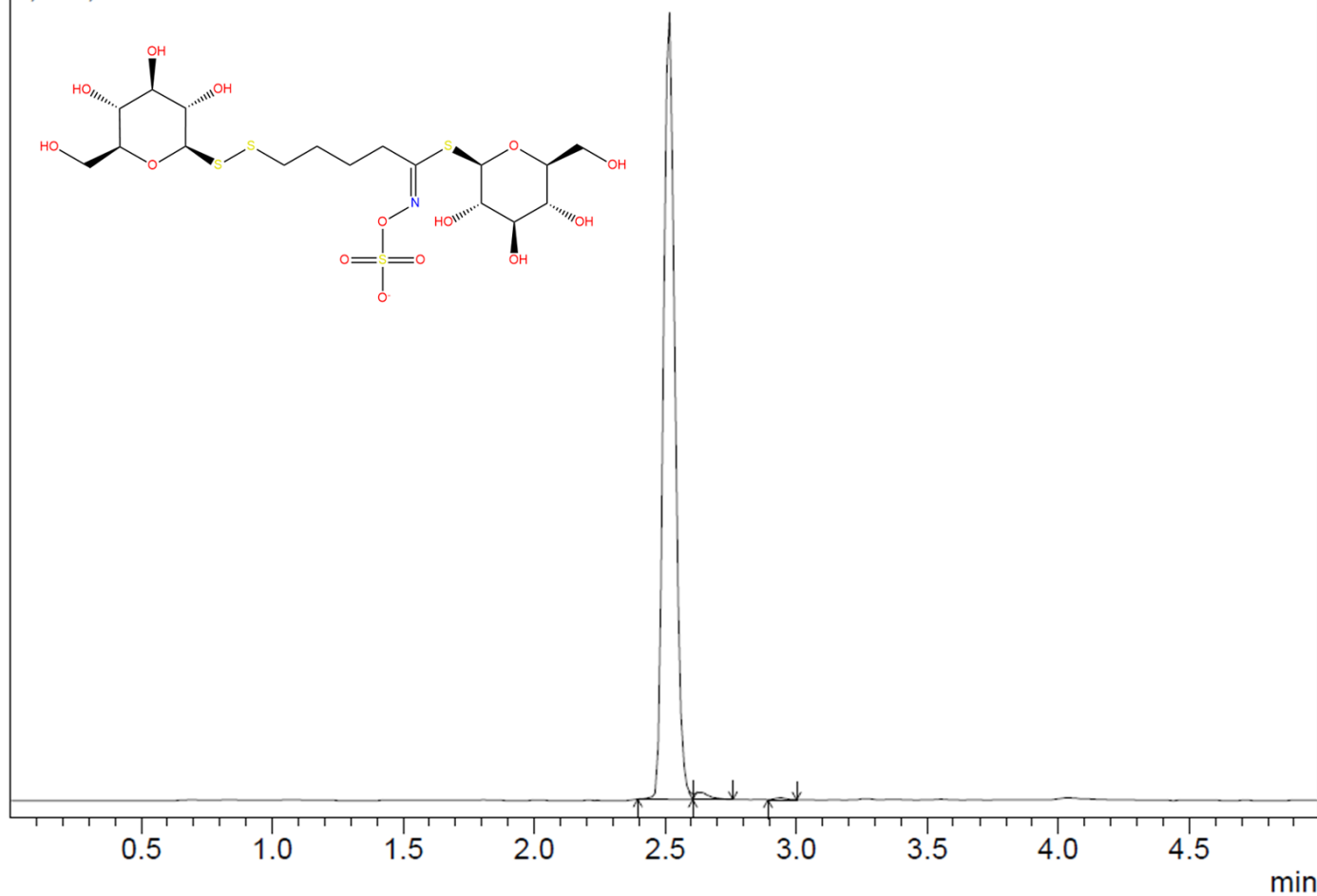


# Gluconapin

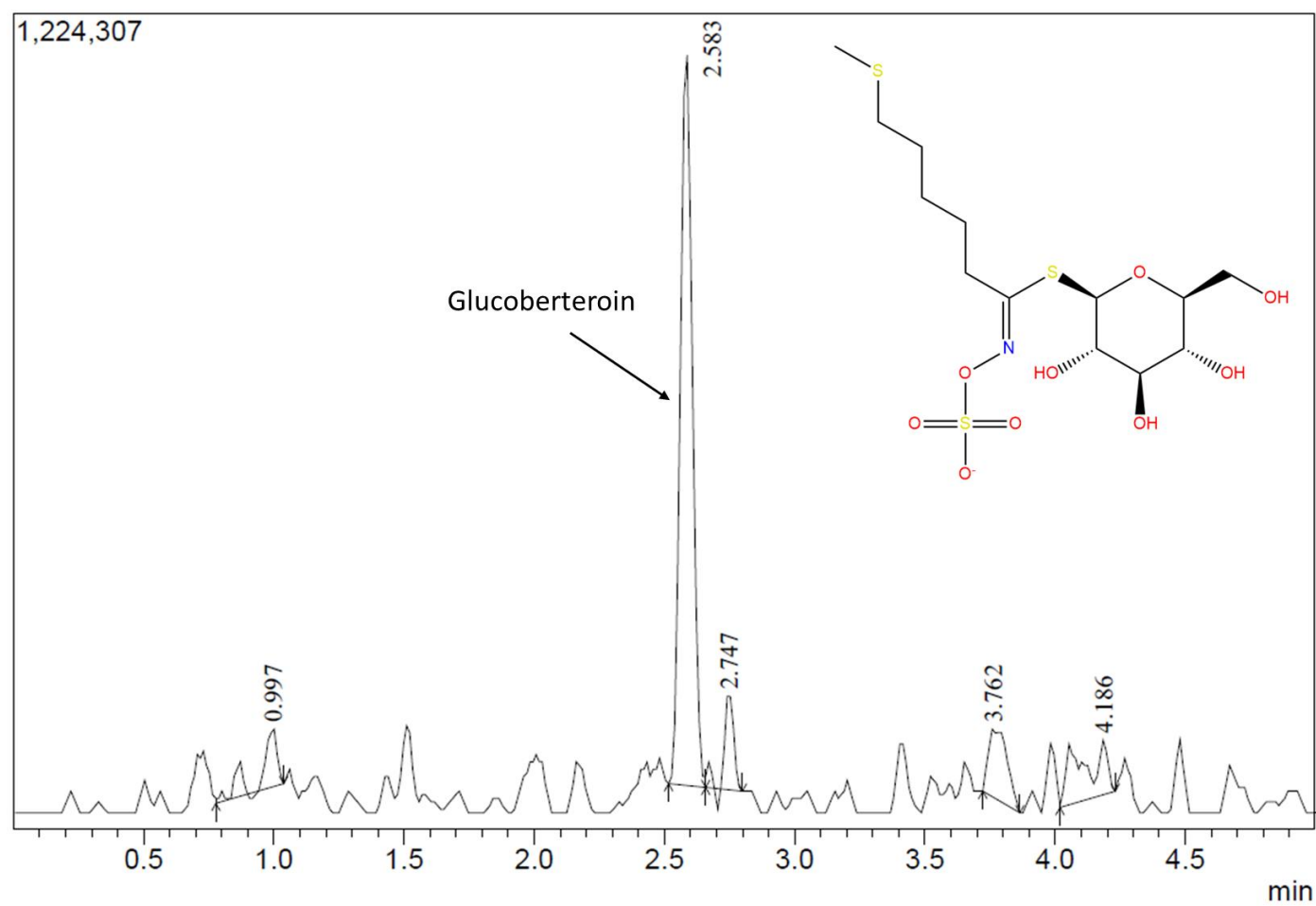


# Diglucothiobeinin

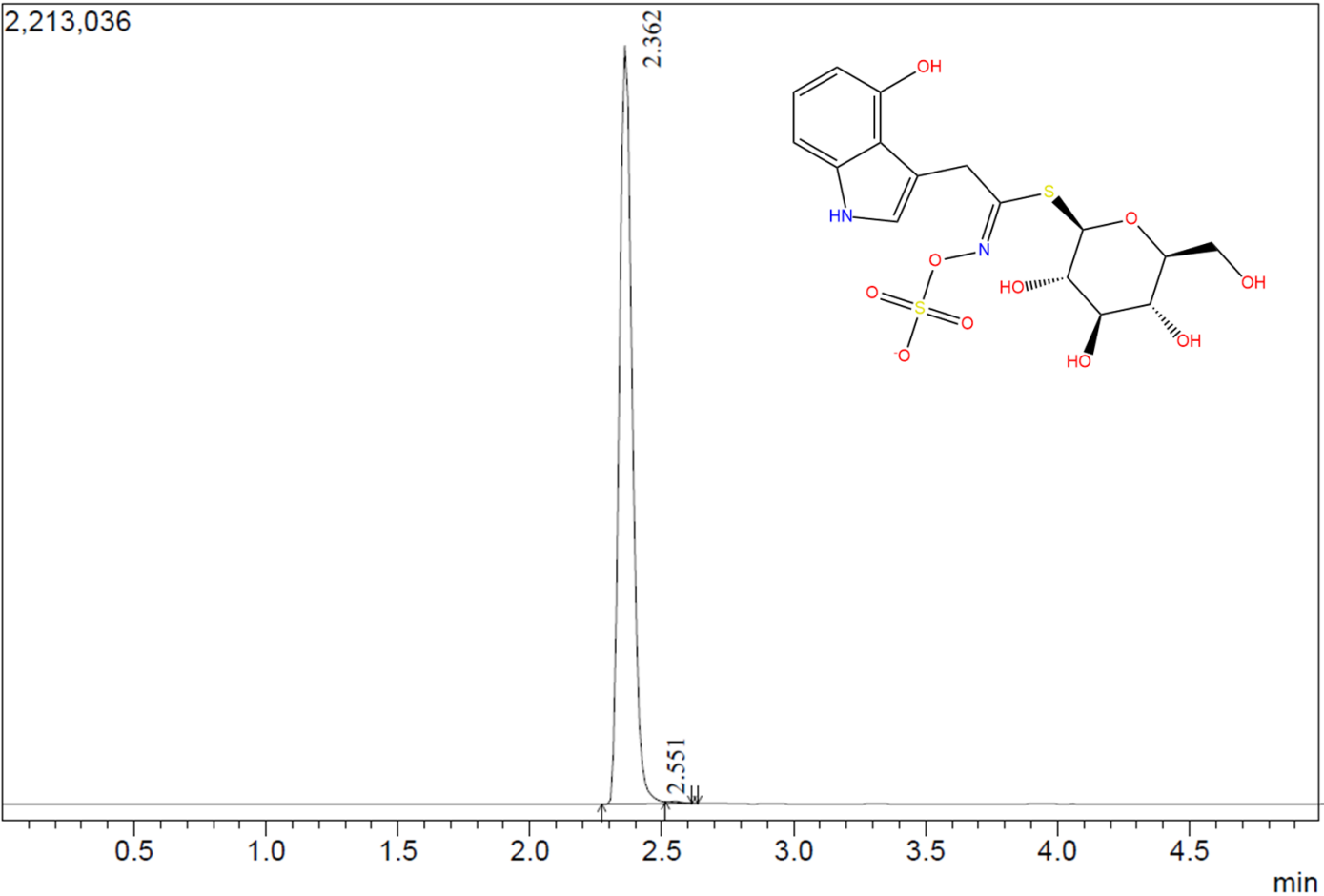
6,267,180



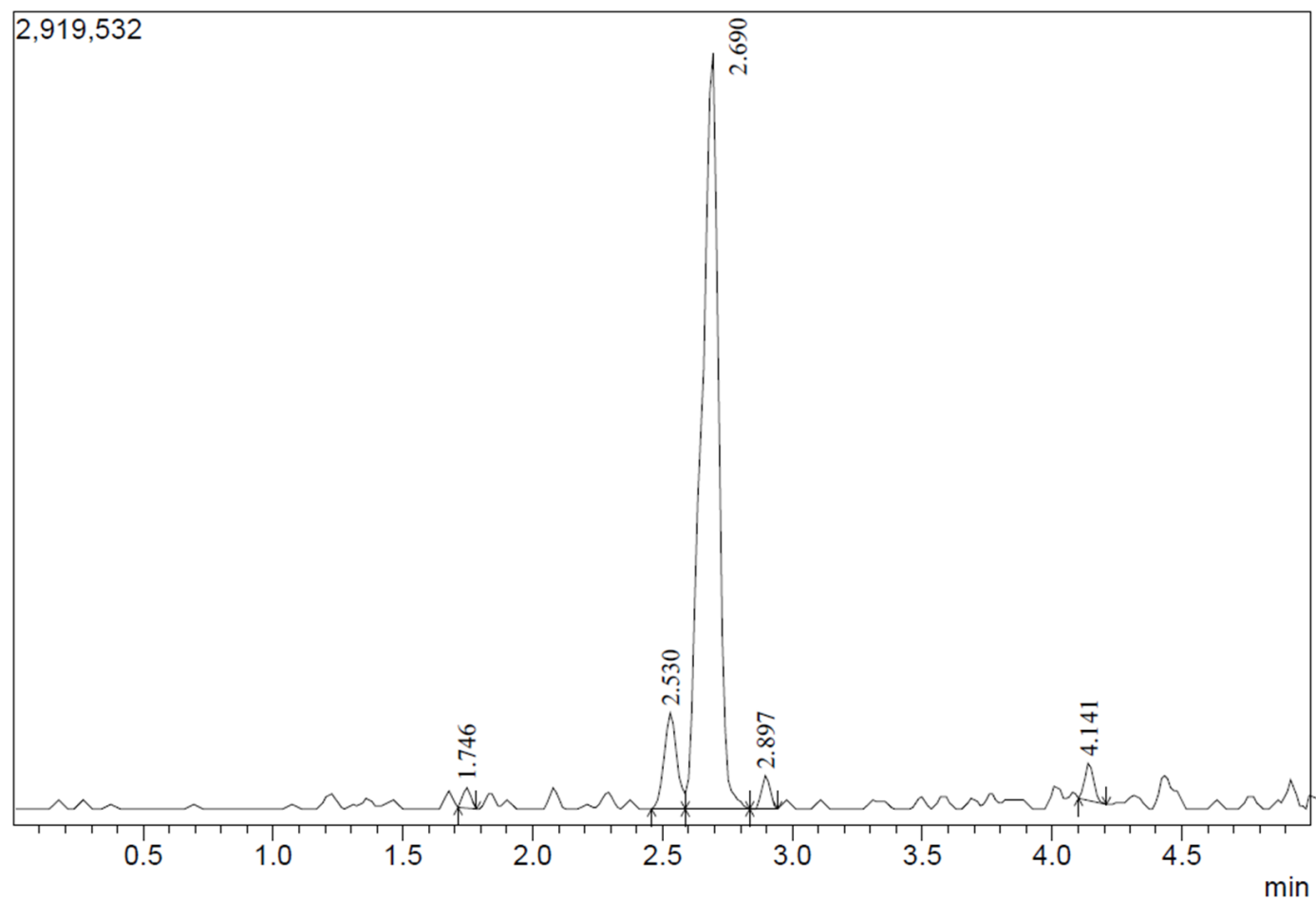
# Glucoberberoin



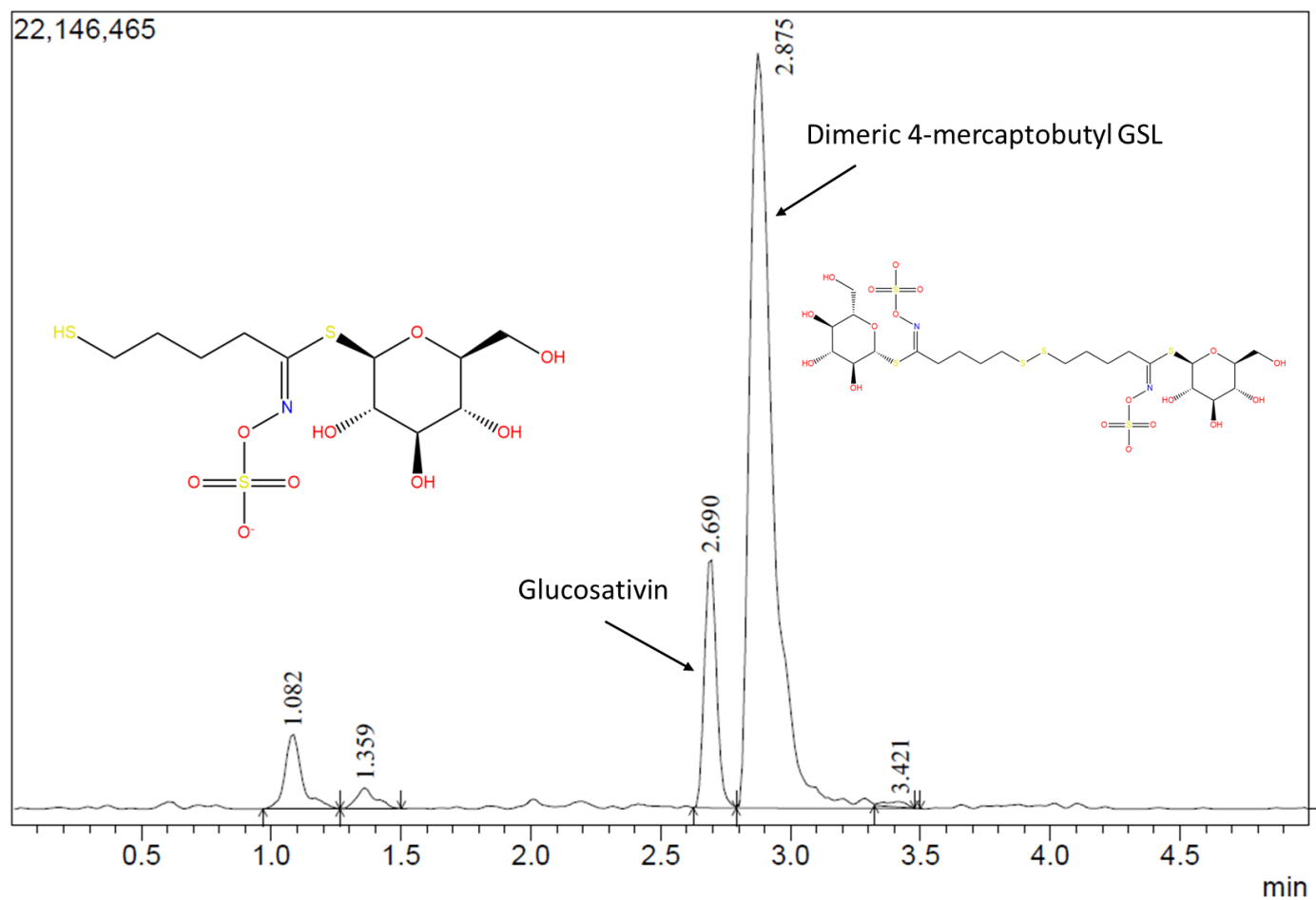
4-hydroxyglucobrassicin



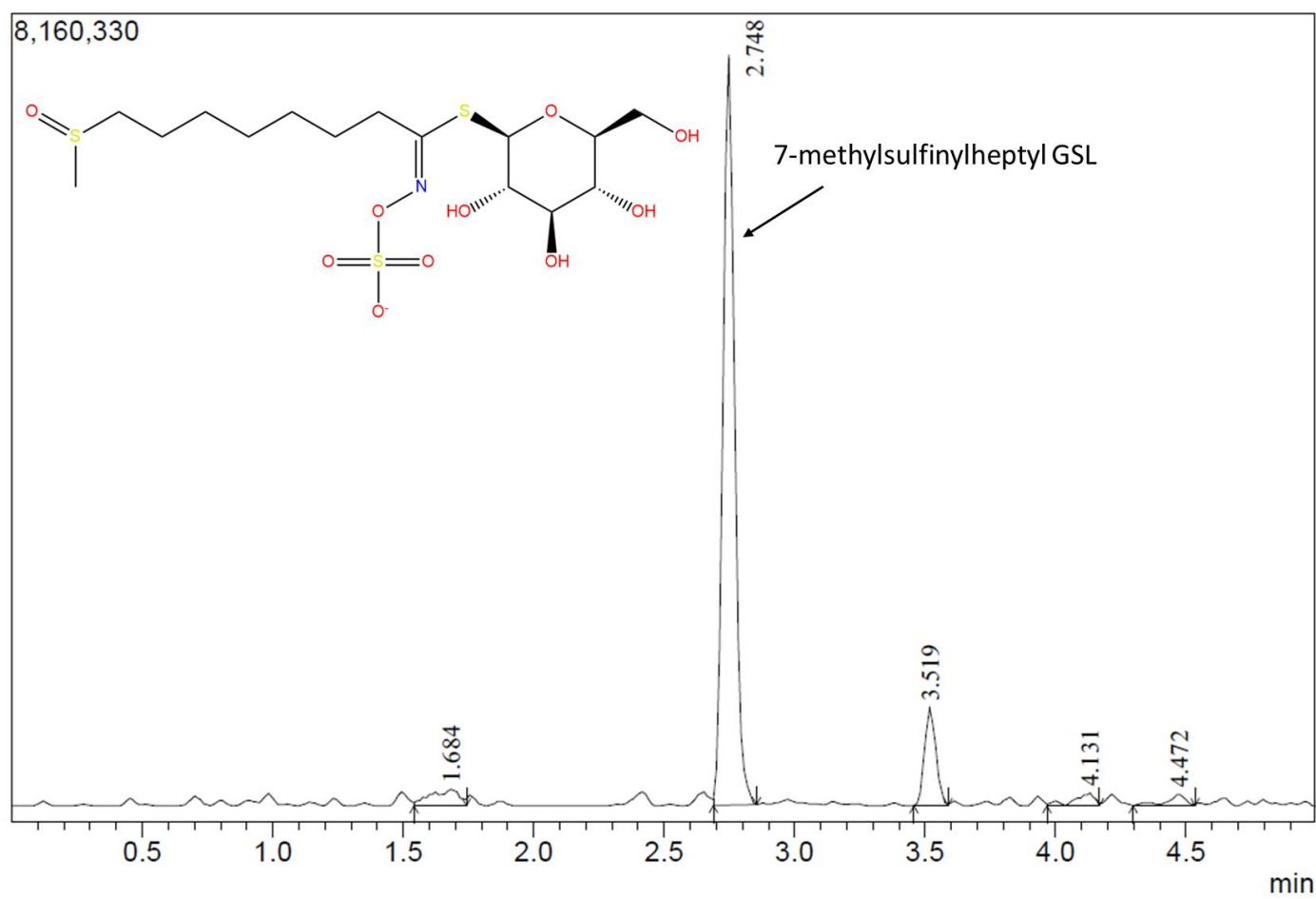
# Glucocochlearin



## Glucosativin & Dimeric 4-mercaptobutyl GSL

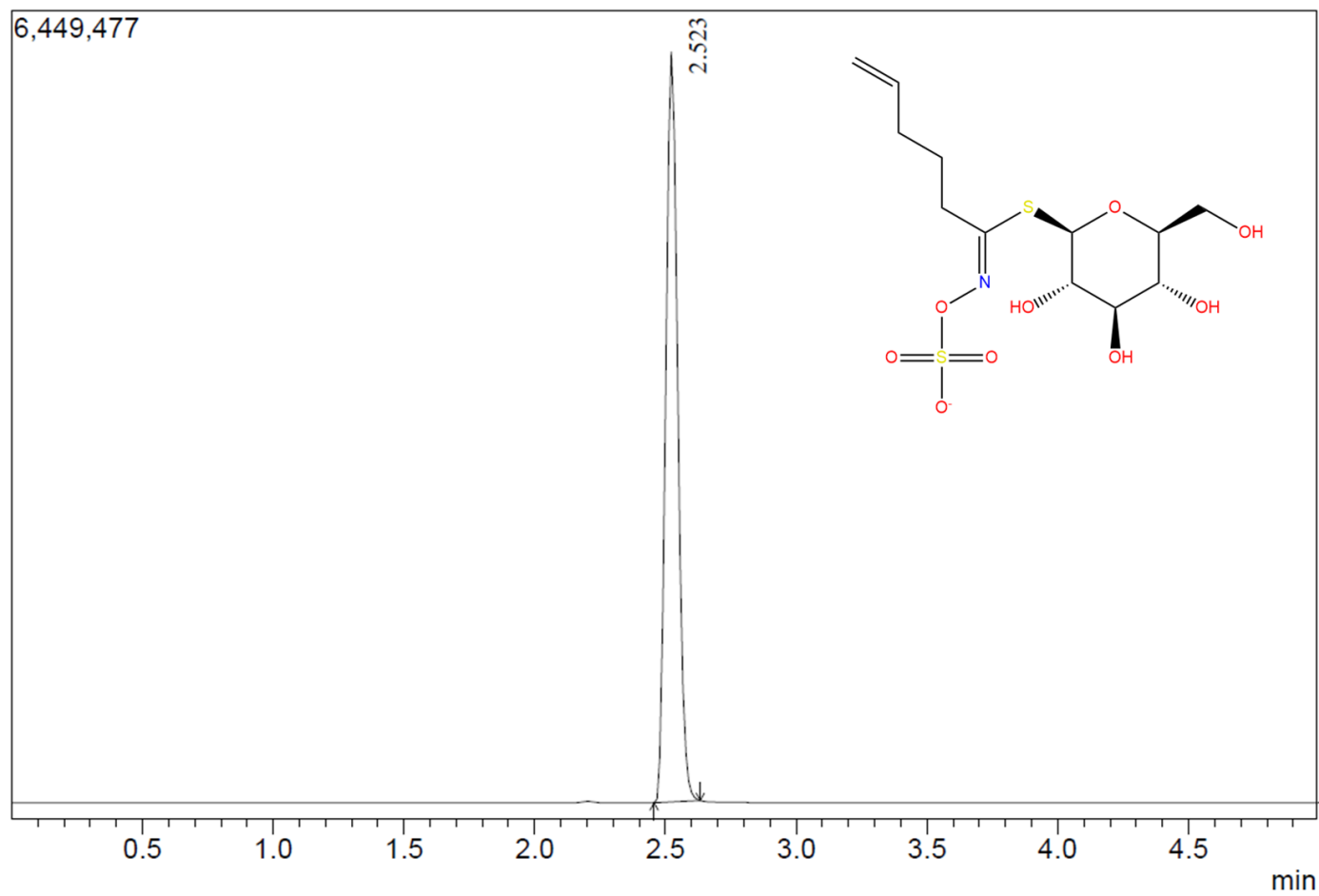


## 7-methylsulfinylheptyl GSL

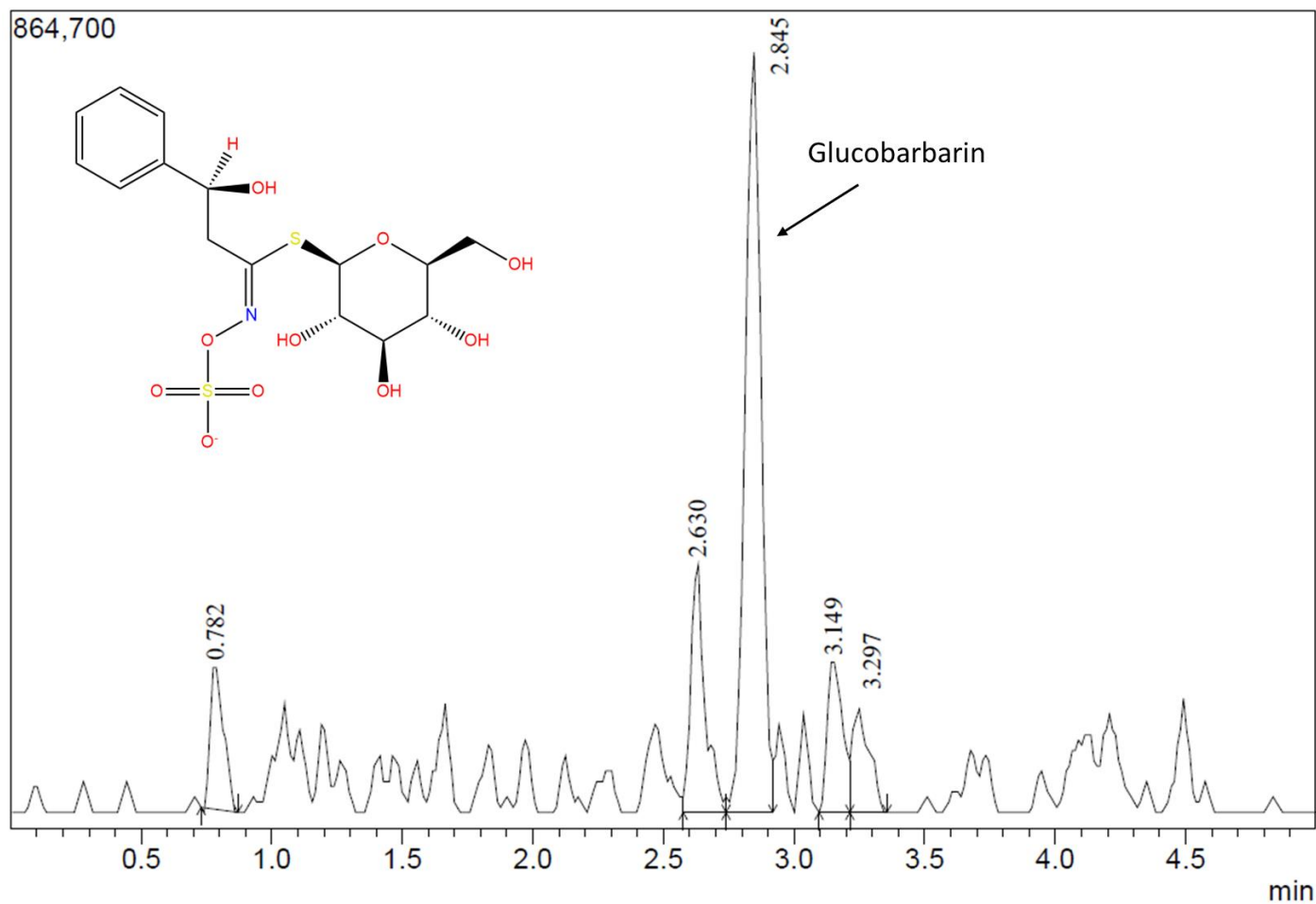




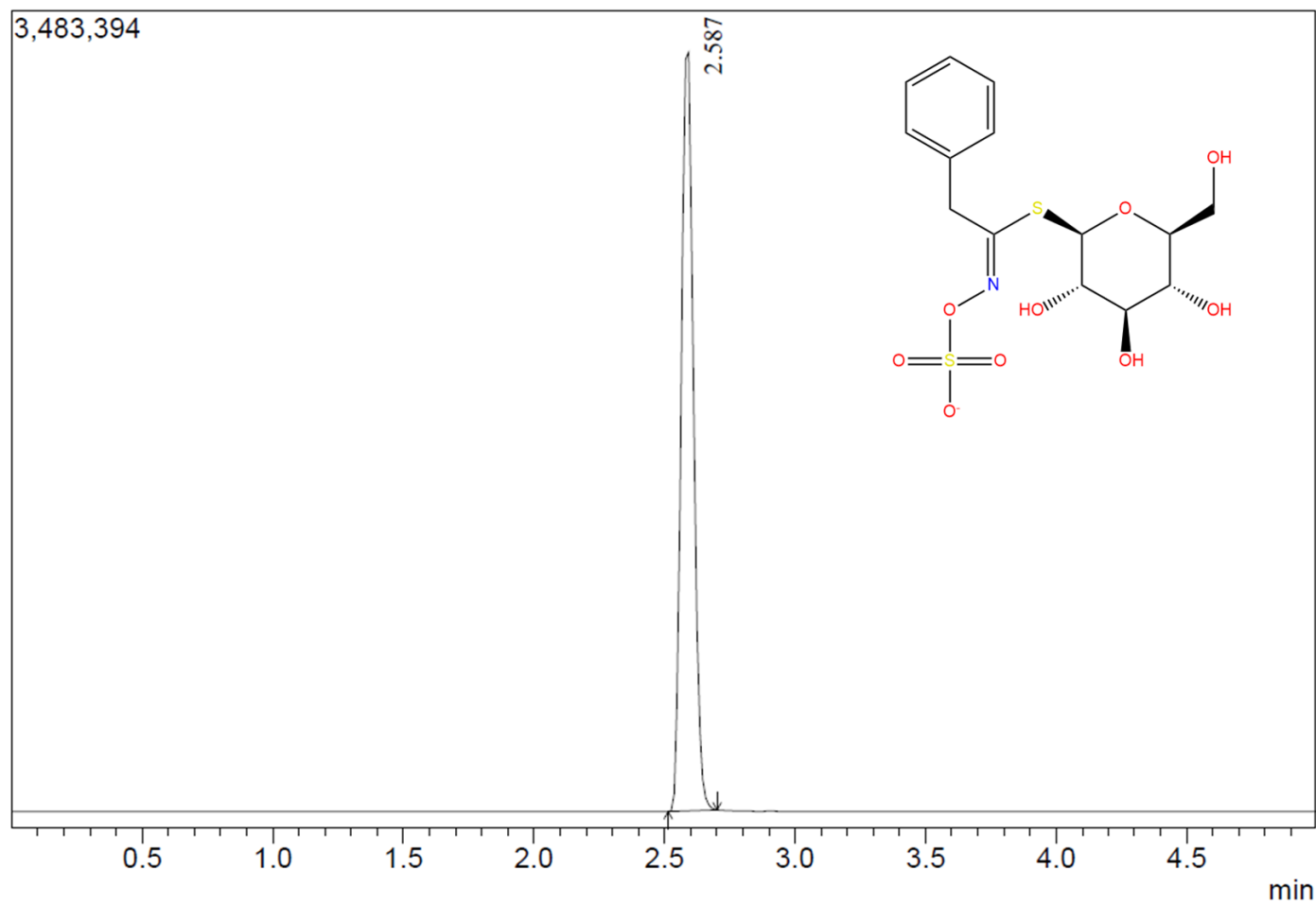
# Glucobrassicinapin



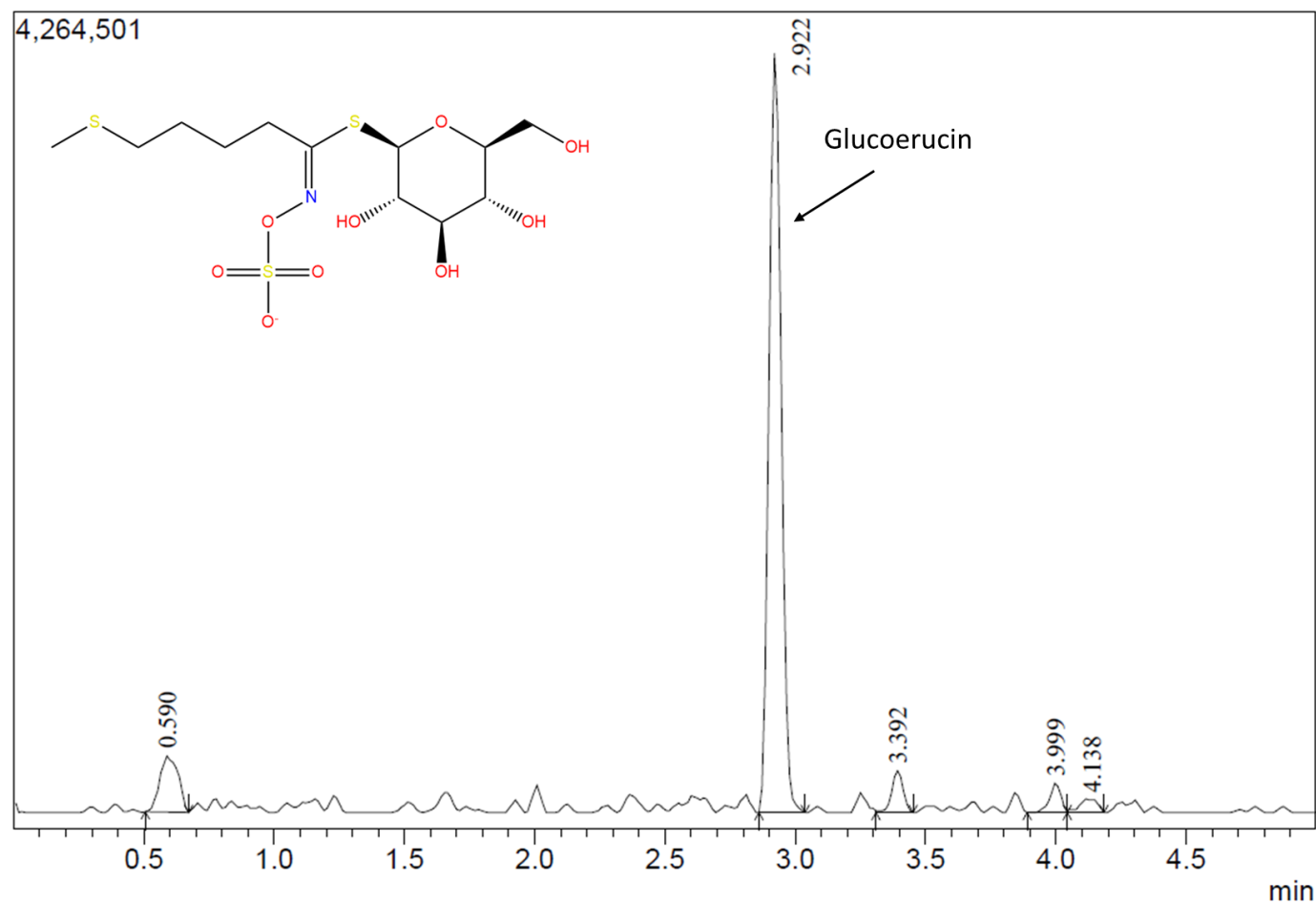
# Glucobarbarin



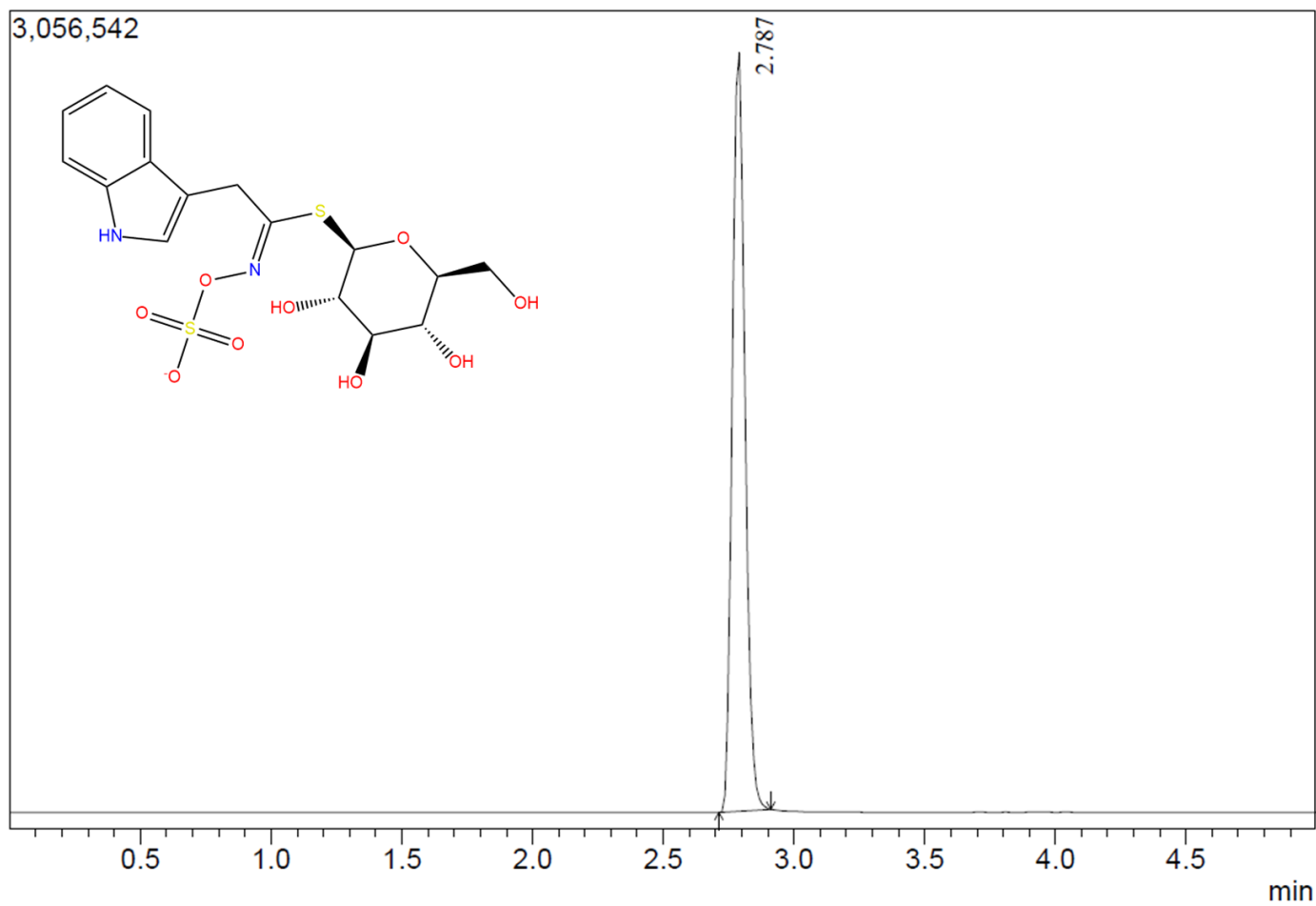
# Glucotropaeolin



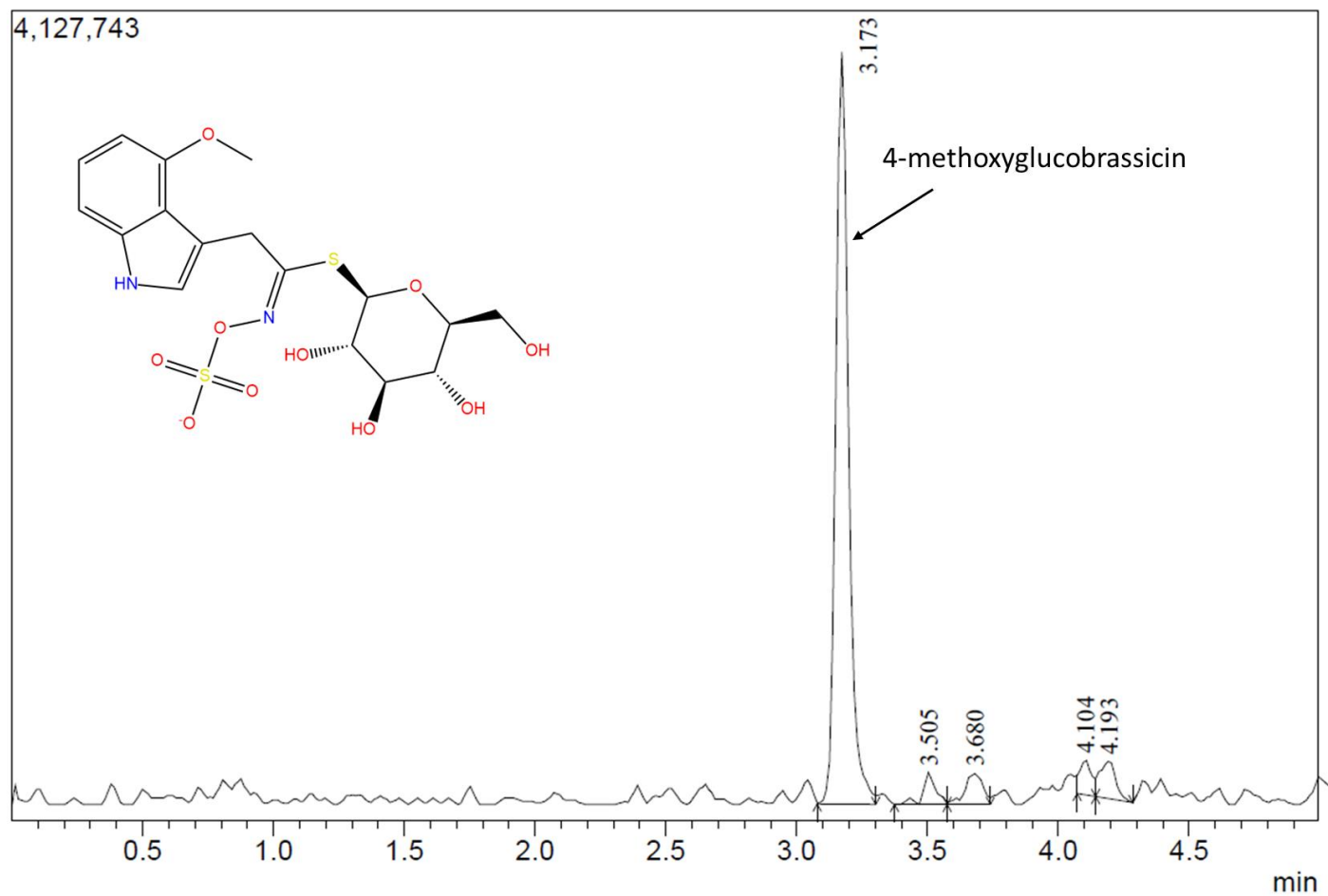
# Glucoerucin



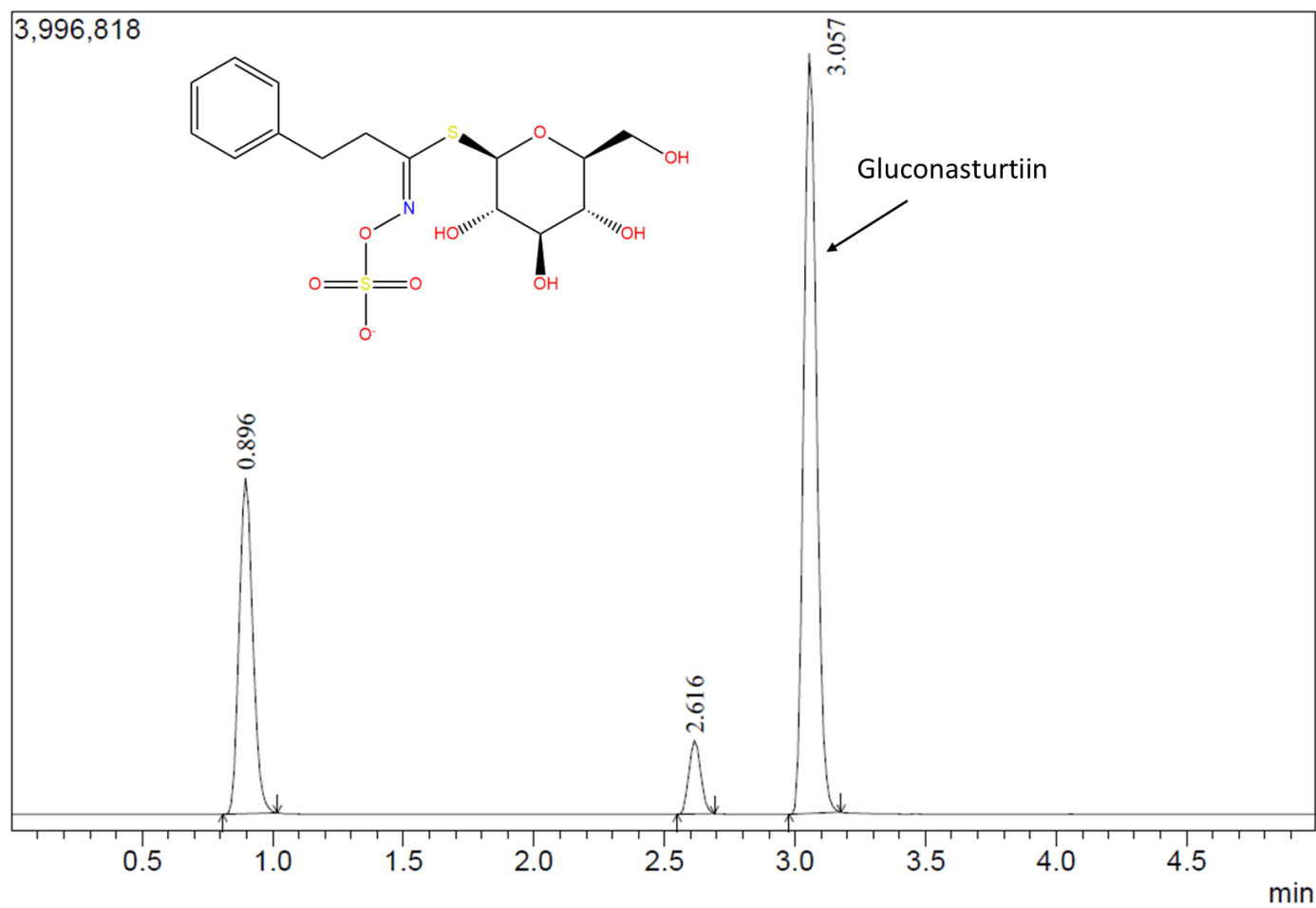
# Glucobrassicin



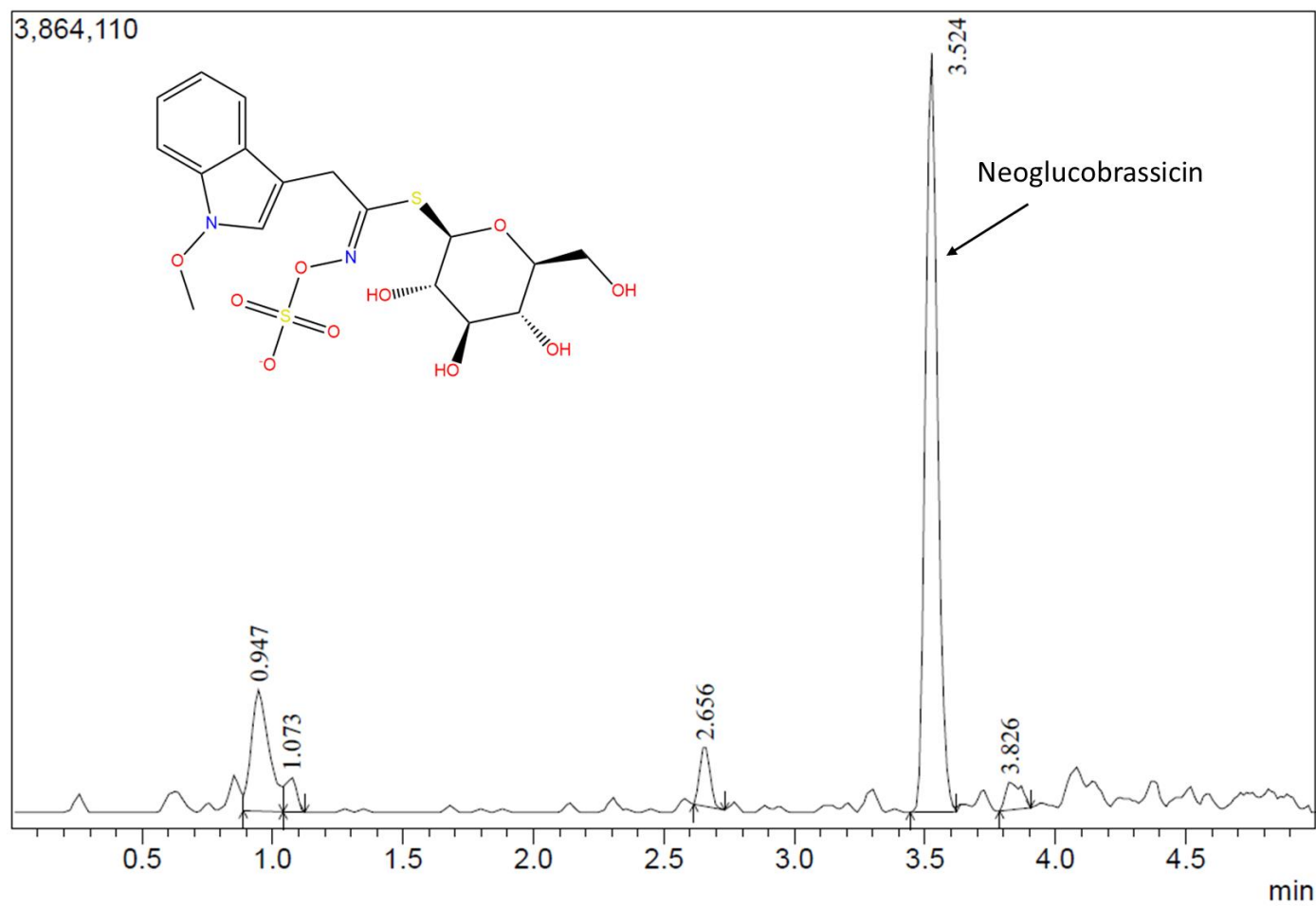
# 4-methoxyglucobrassicin



# Gluconasturtiin

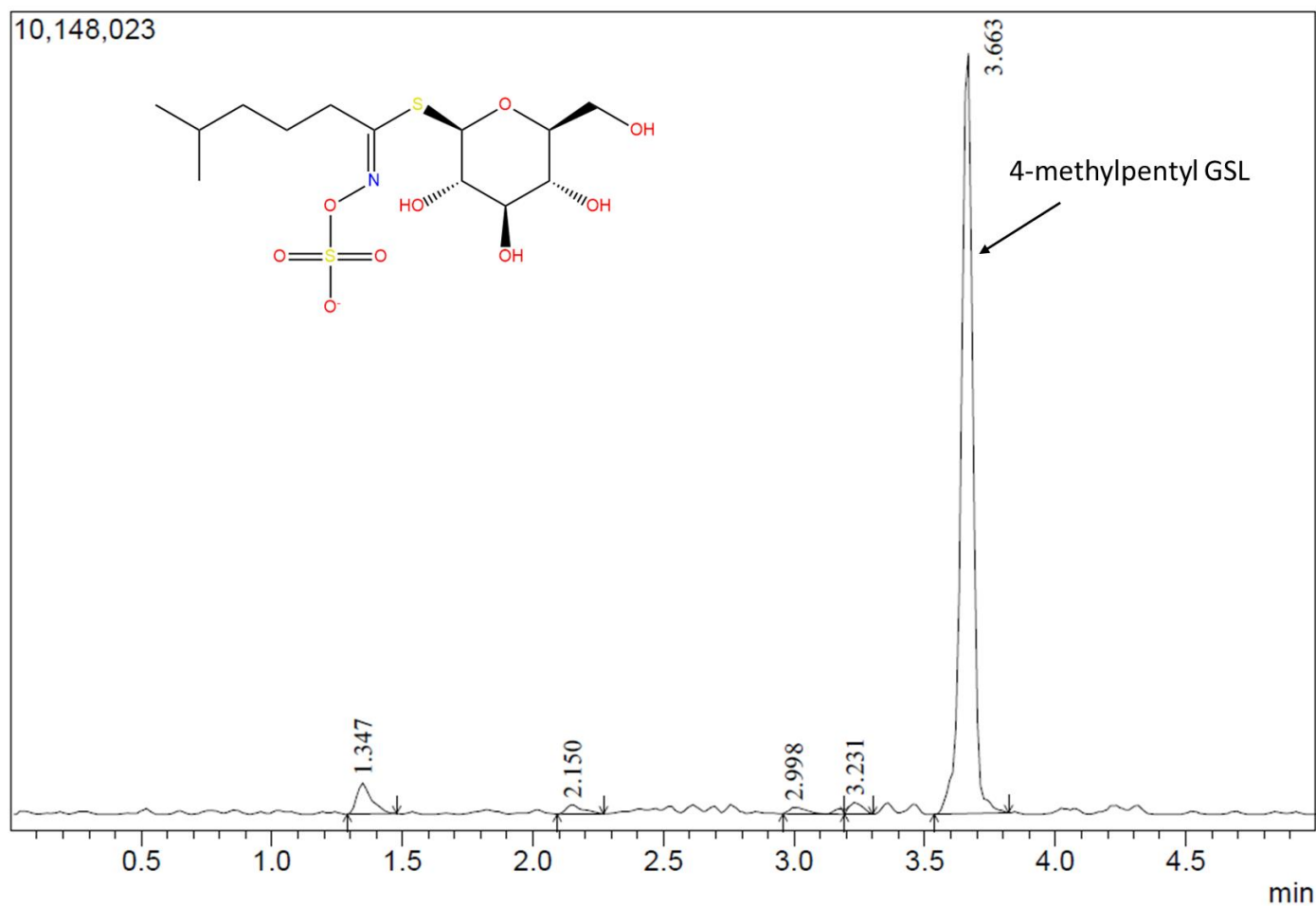


# Neoglucobrassicin

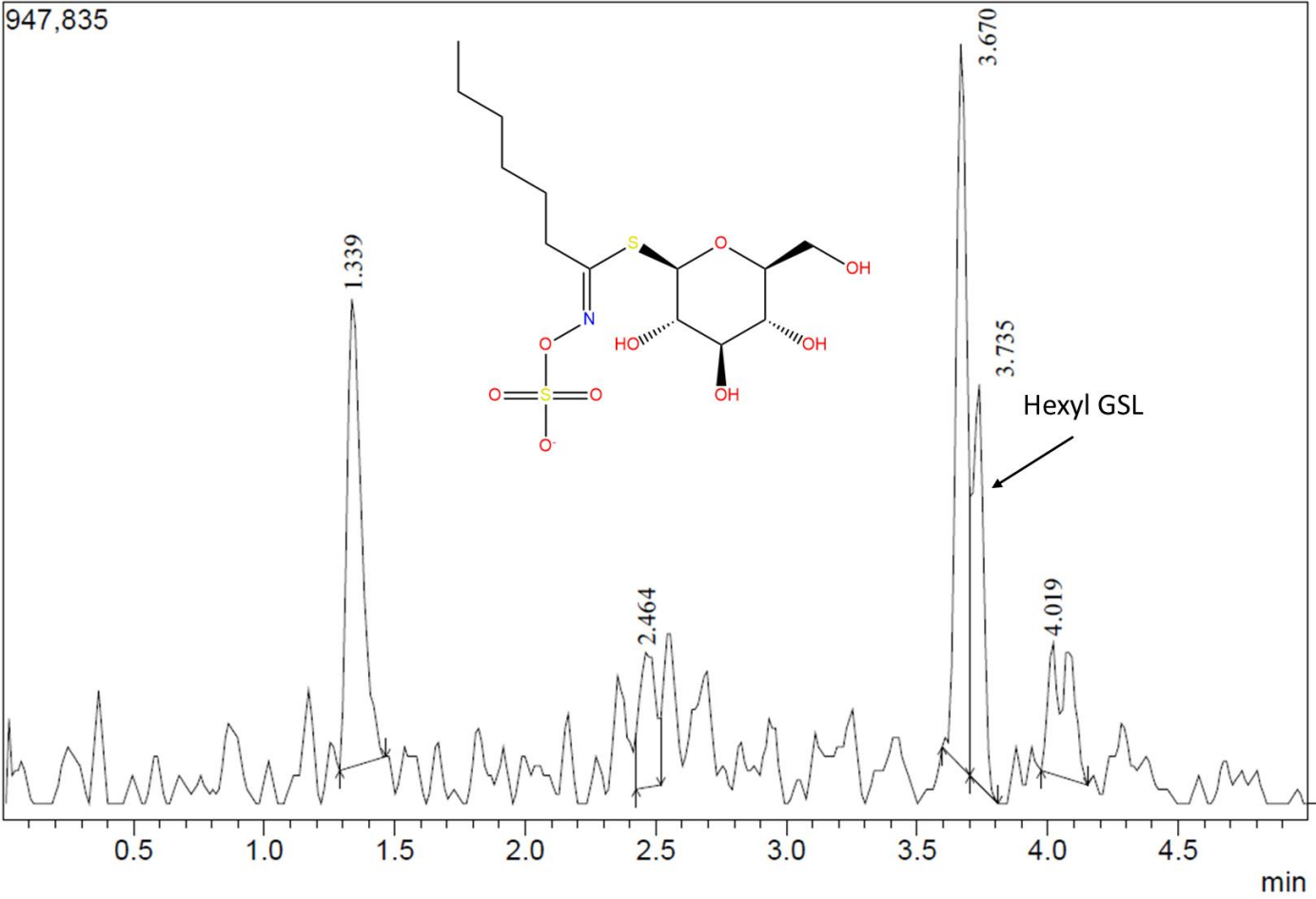




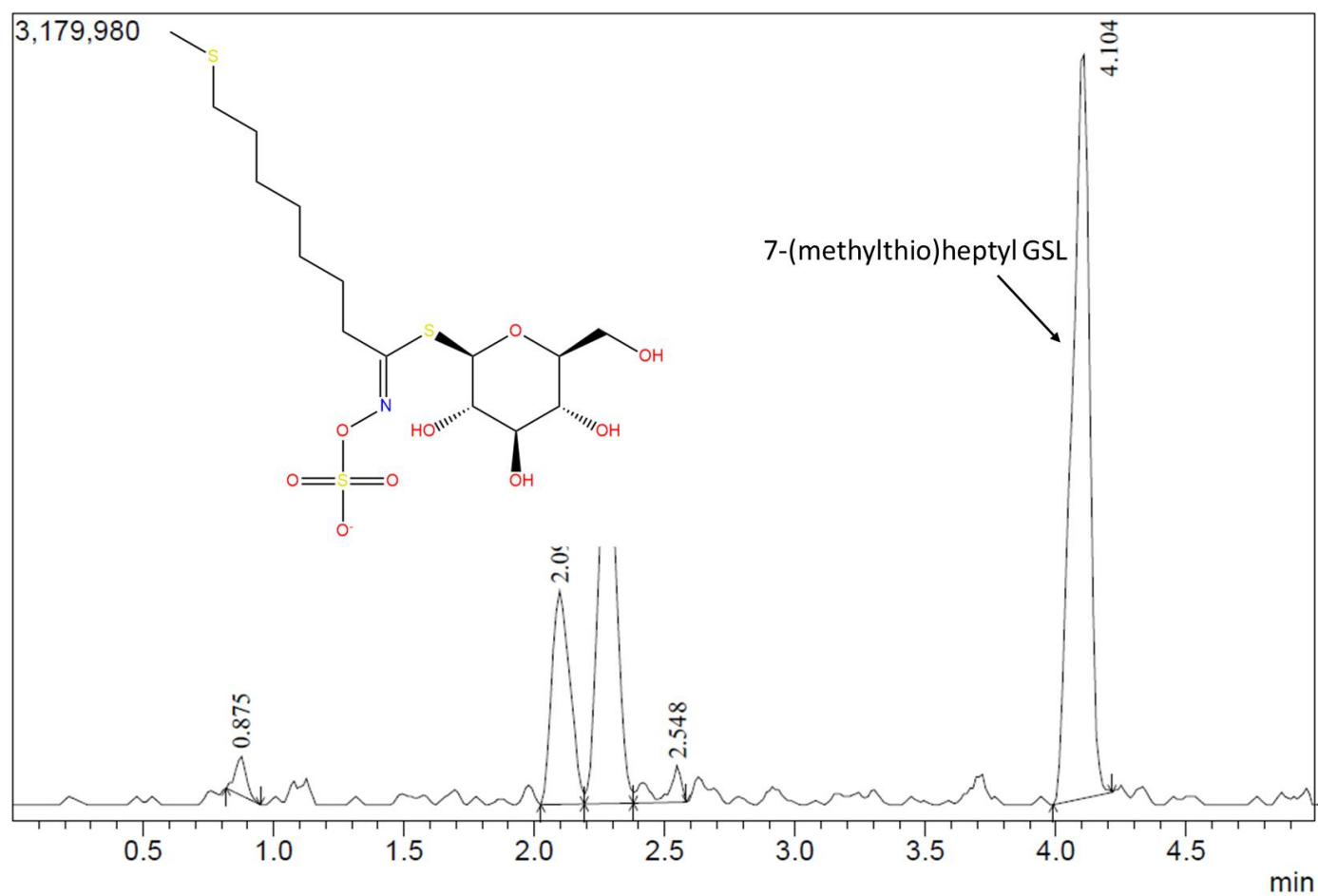
## 4-methylpentyl GSL



Hexyl GSL



# 7-(methylthio)heptyl GSL



# Butyl GSL

