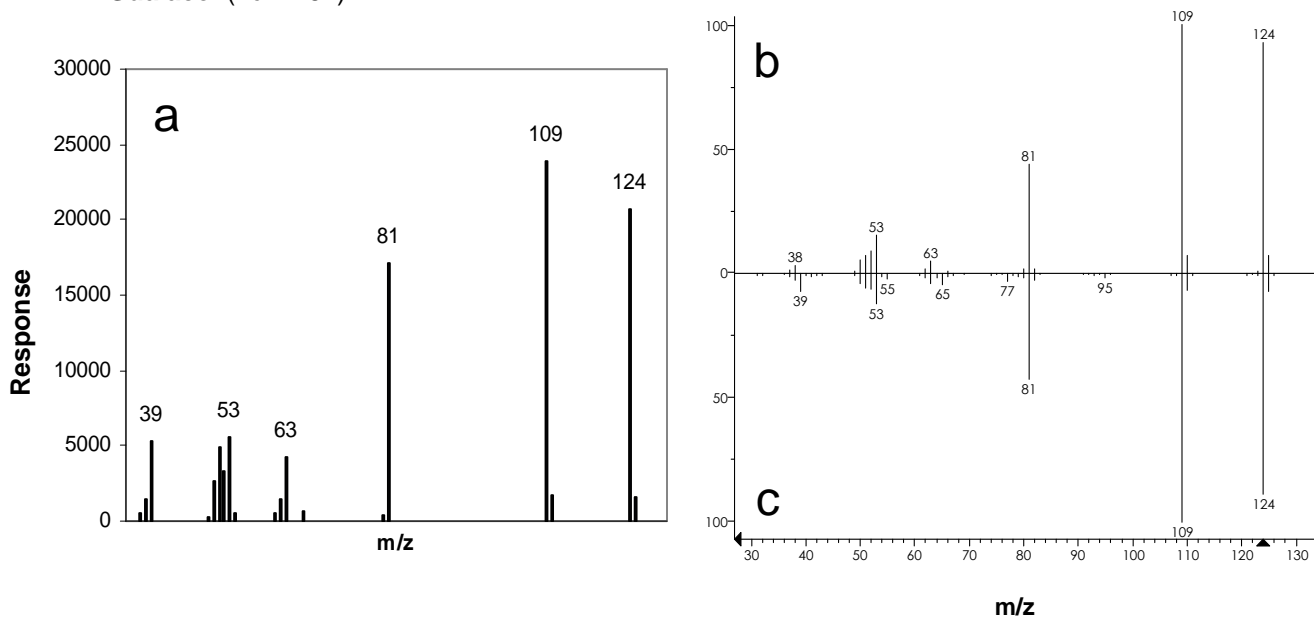


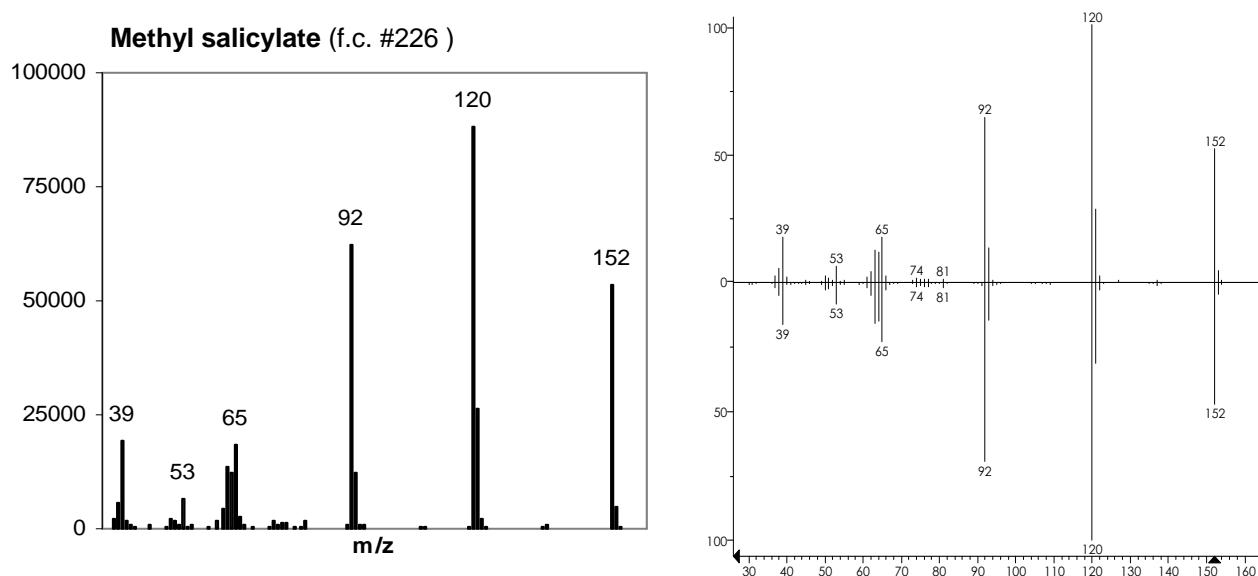
Supplemental data II. Correspondence of fragment clusters (f.c.) derived by MMSR to mass spectral characteristics of the tomato fruit volatiles.

The 70 compounds shown in Table II of the text are presented. **a)** Mass spectrum reconstructed by MMSR: original intensities (Response) of fragments (ions, m/z) plotted as an Excel chart; **b)** mass spectral model extracted from a GC/MS profile using AMDIS deconvolution based on MMSR results as described in the Materials and Methods; **c)** mass spectrum of the first matching hit derived from the NIST library for the mass spectral model obtained by the AMDIS deconvolution on **(b)**.

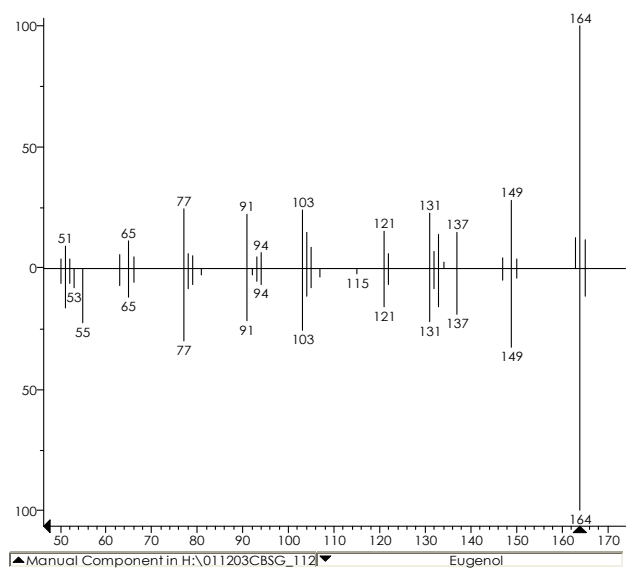
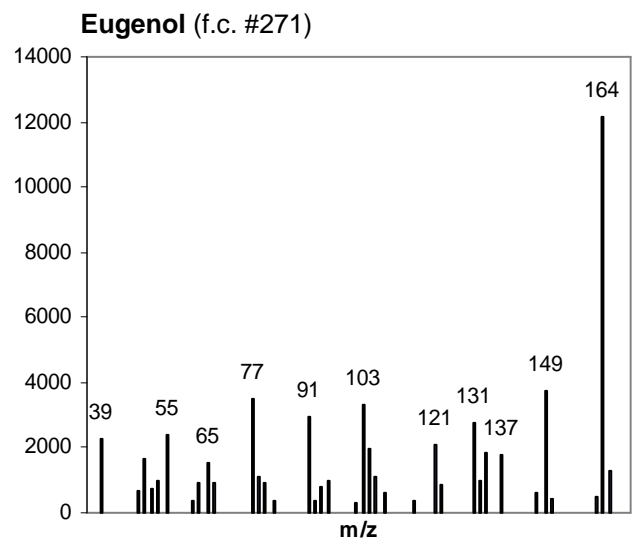
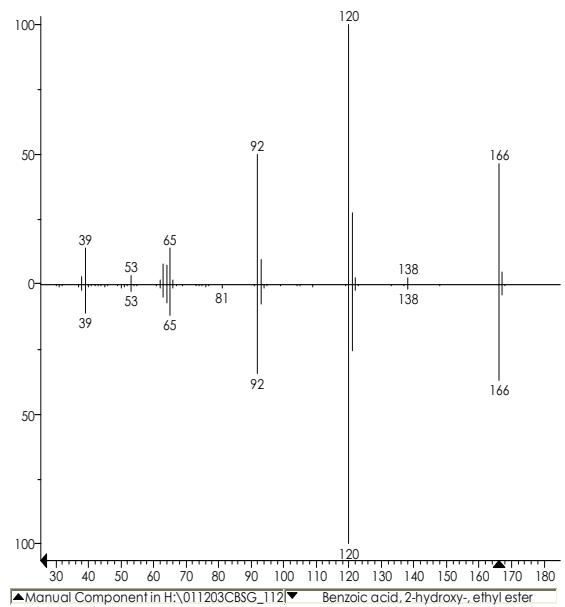
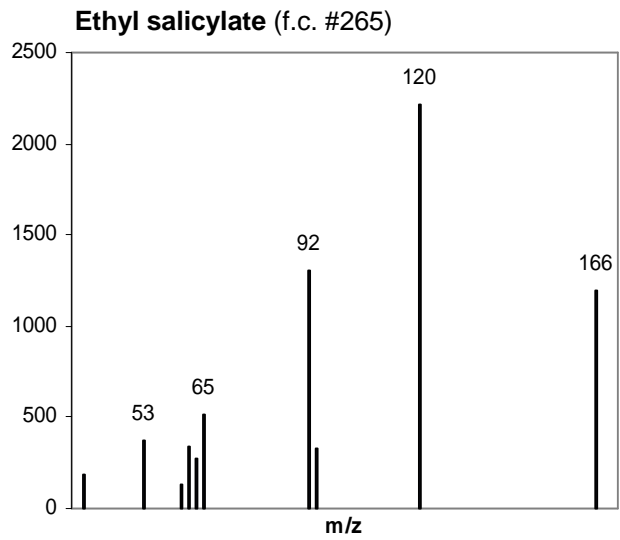
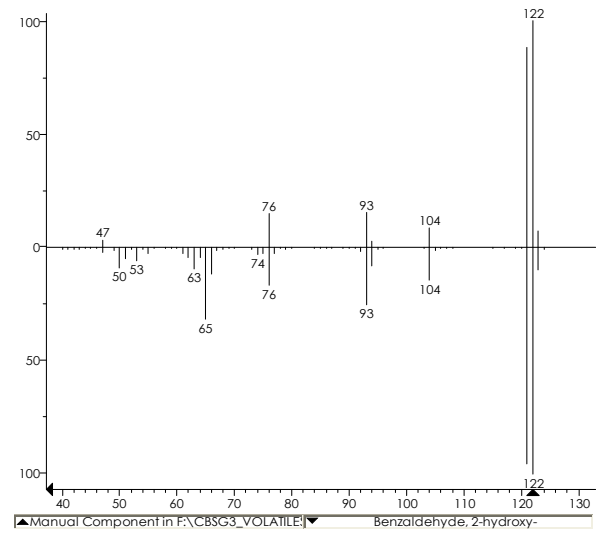
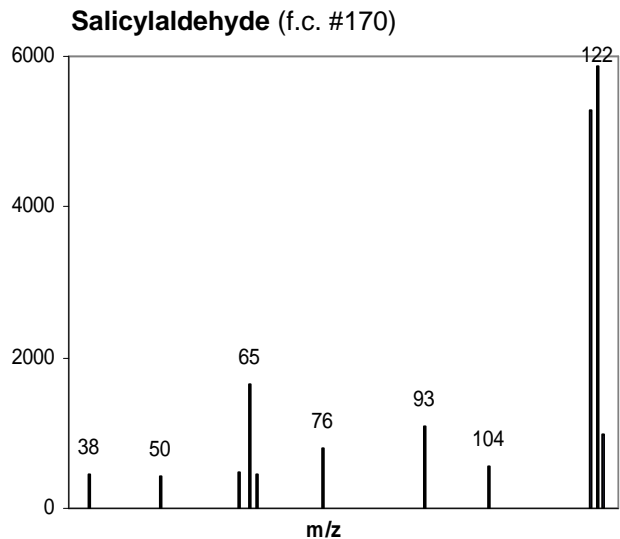
Guaiacol (f.c. #162)*



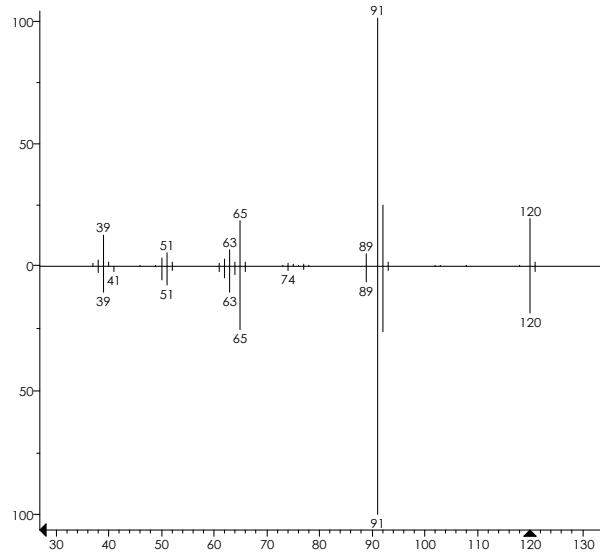
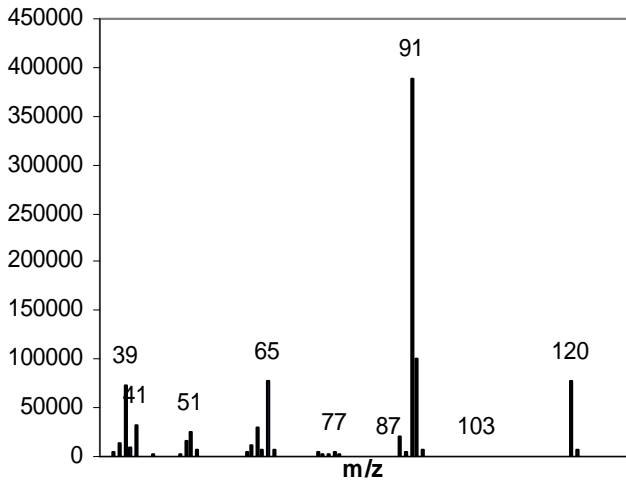
Methyl salicylate (f.c. #226)



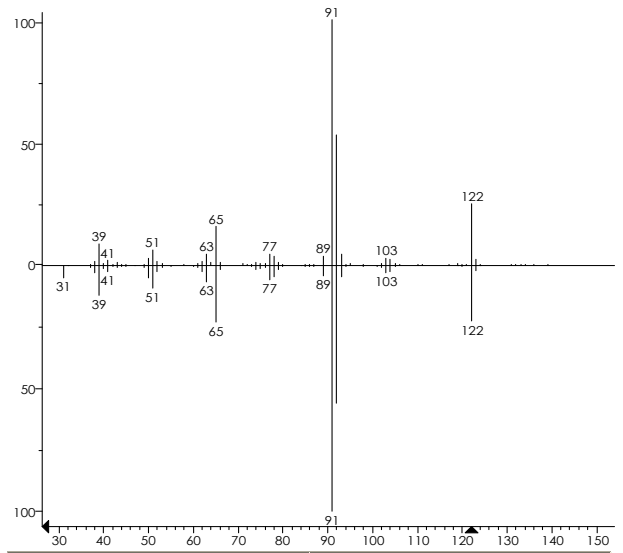
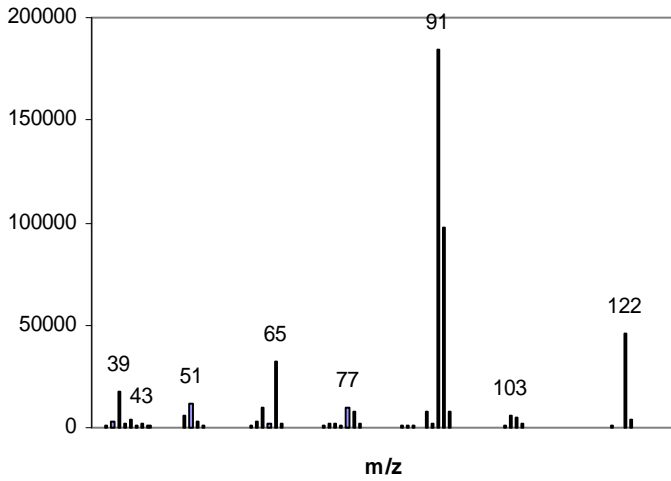
* Number of a fragment cluster in the MMSR results



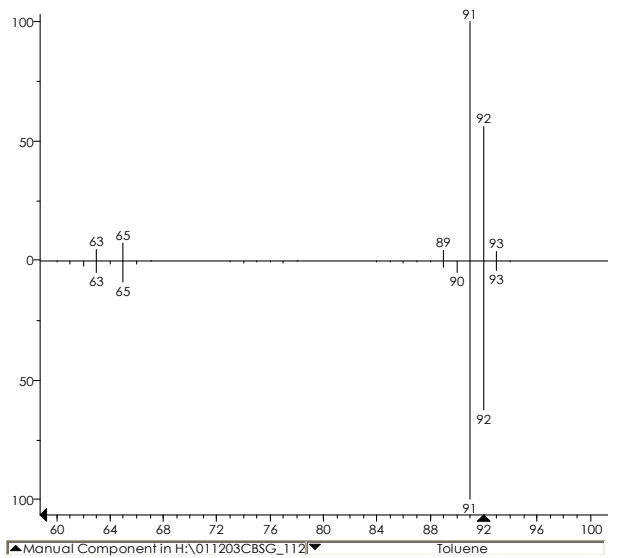
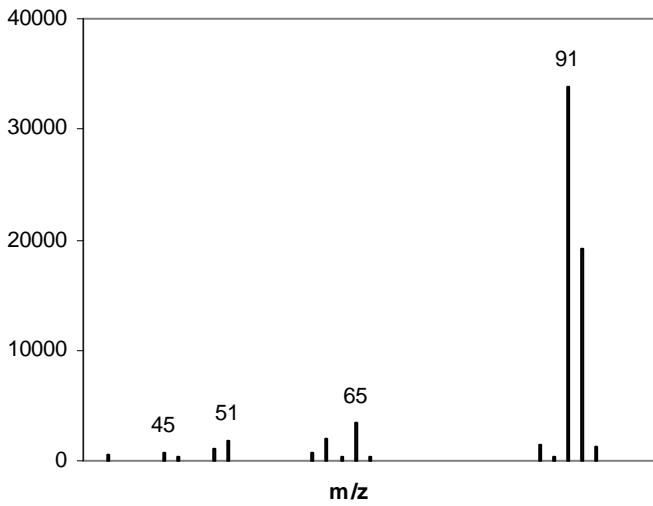
Phenylacetaldehyde (f.c. #152)



Phenylethanol (f.c. #199)



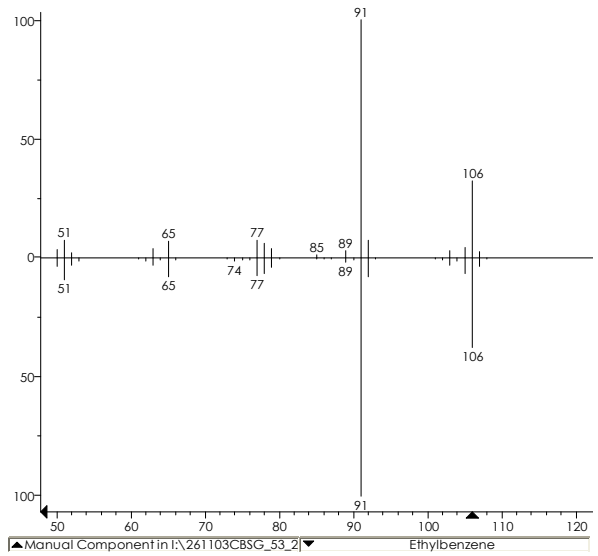
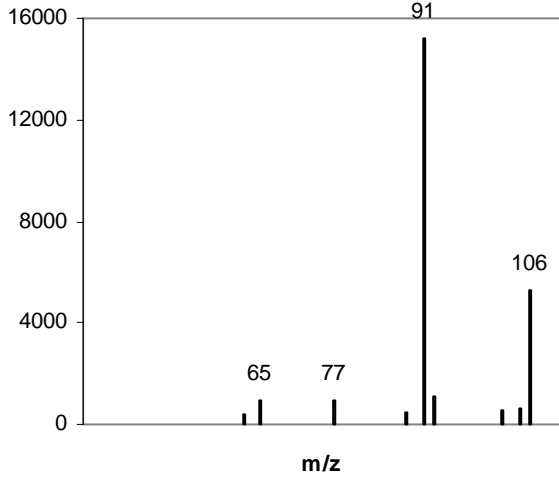
Toluen (f.c. #34)



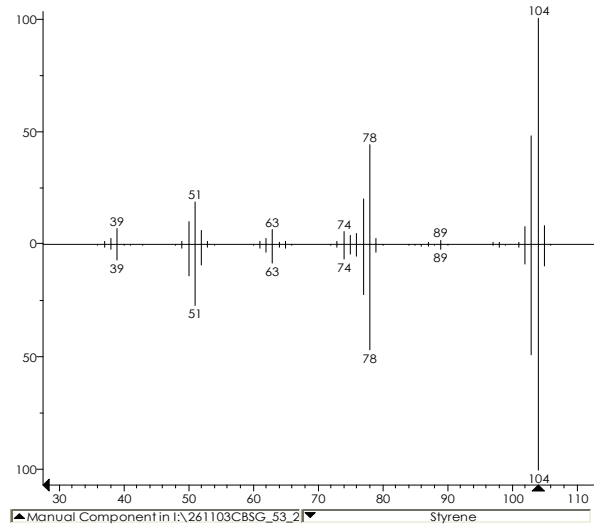
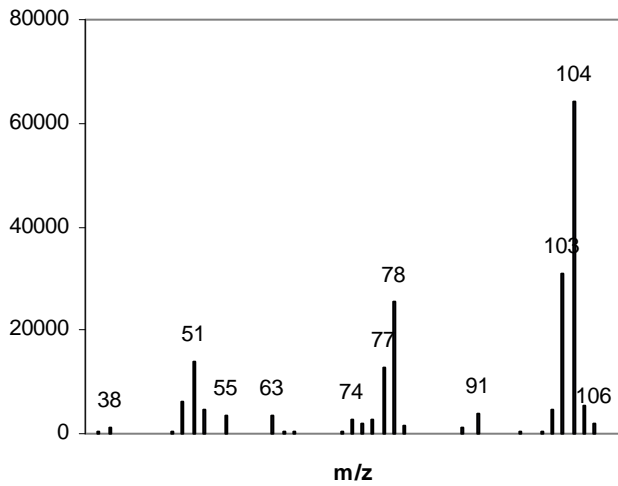
Manual Component in H:\011203CBSG_112

Toluene

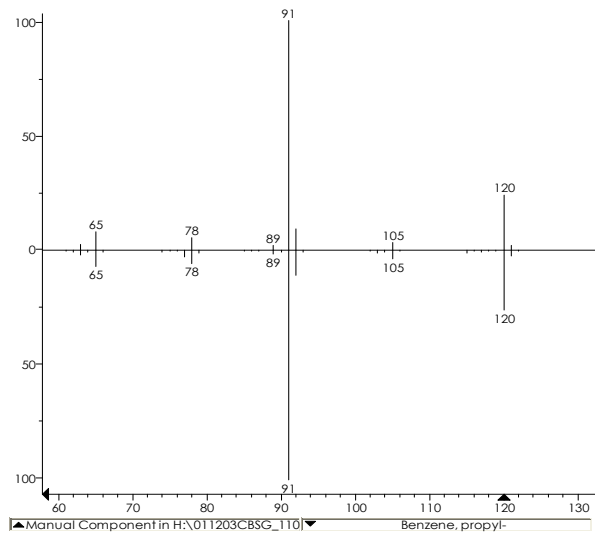
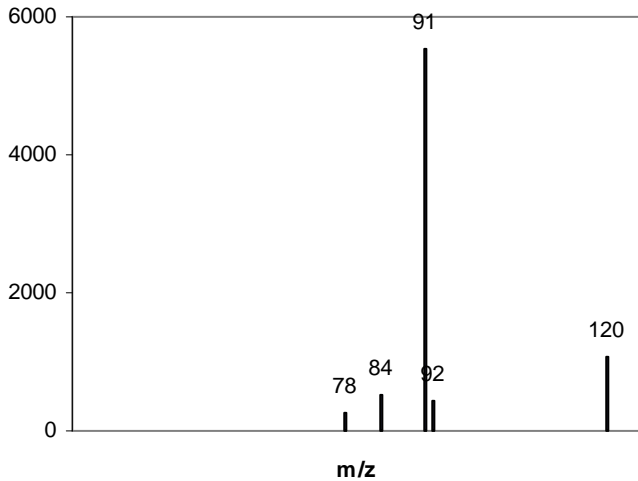
Ethyl benzen (f.c. #67)



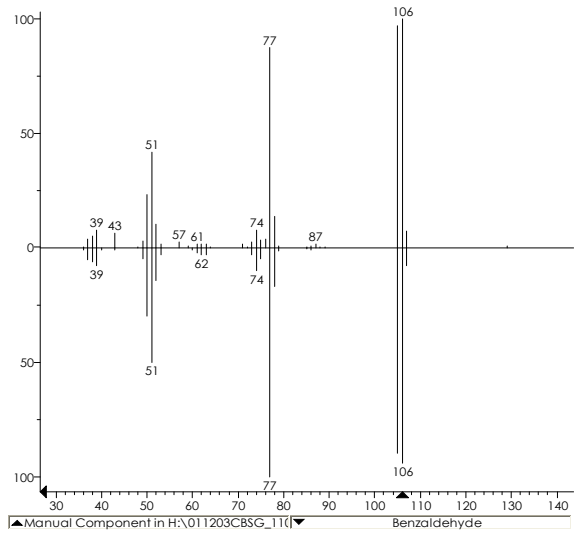
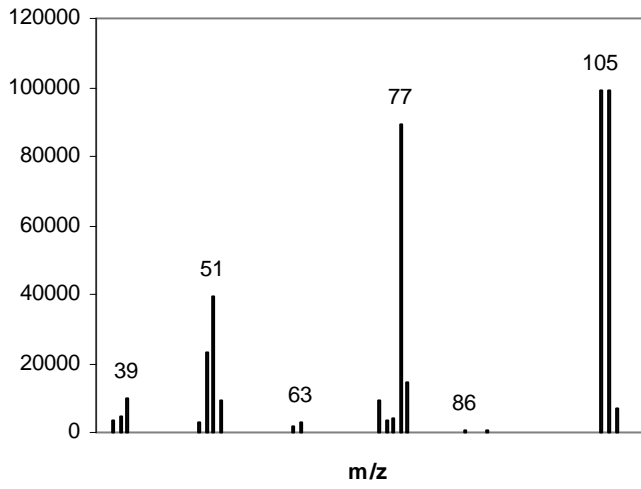
Styren (f.c. #66)



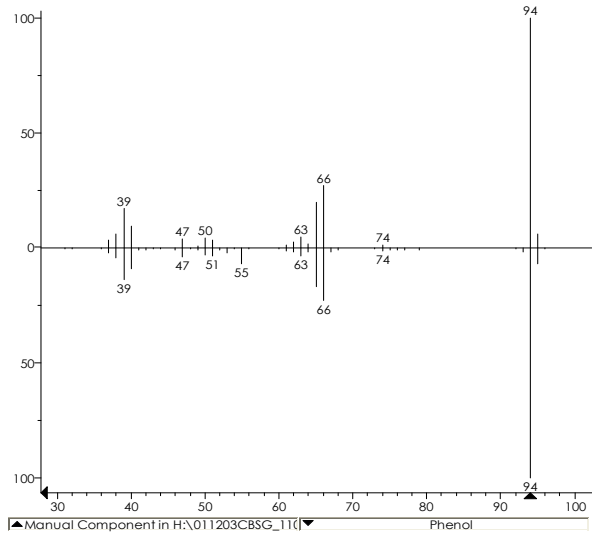
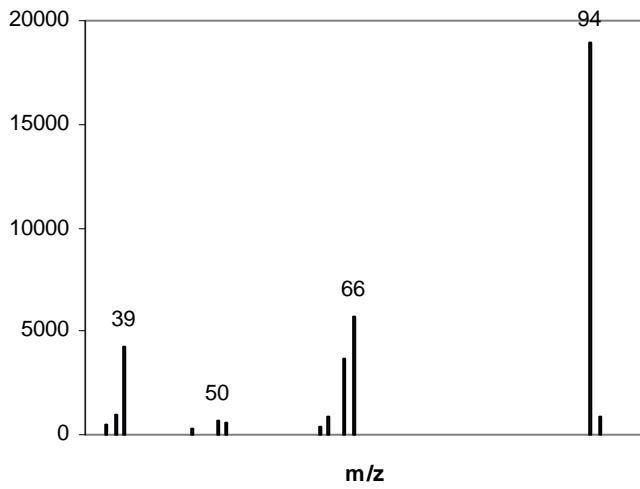
1-Phenylpropane (f.c. #102)



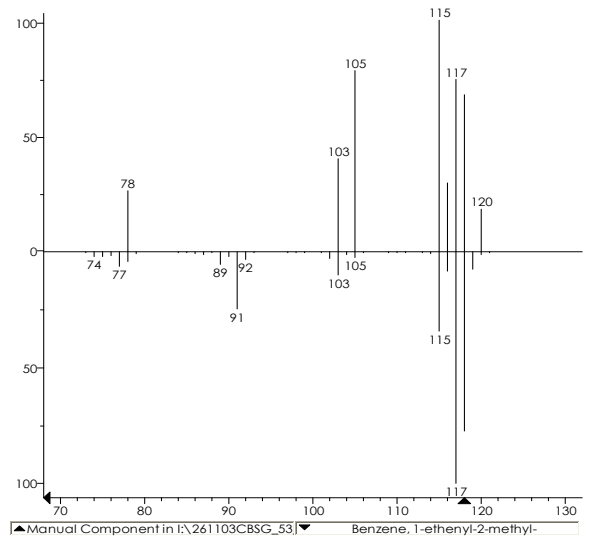
Benzaldehyde (f.c. #103)



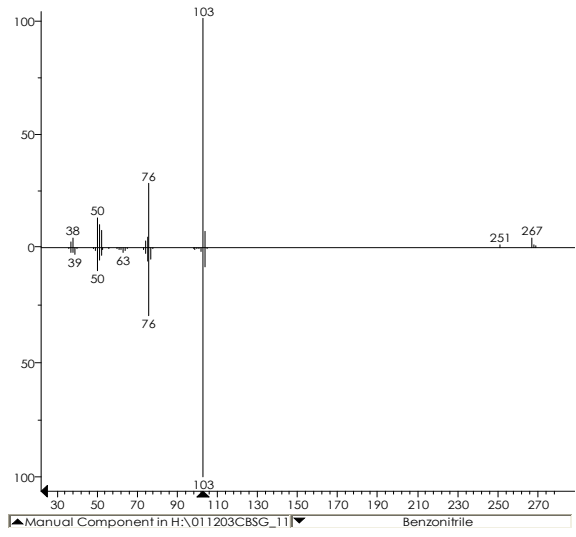
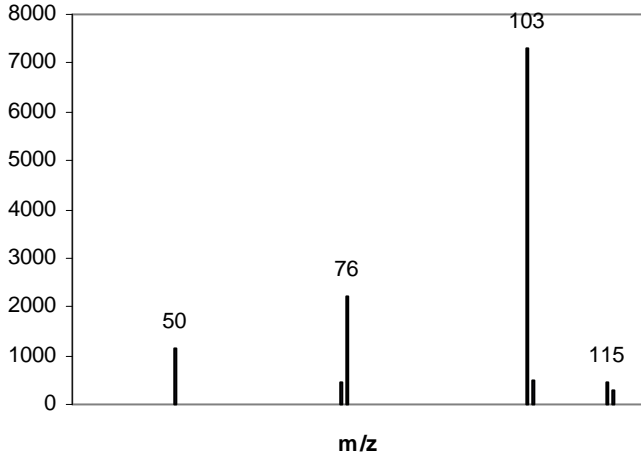
Phenol (f.c. #106)



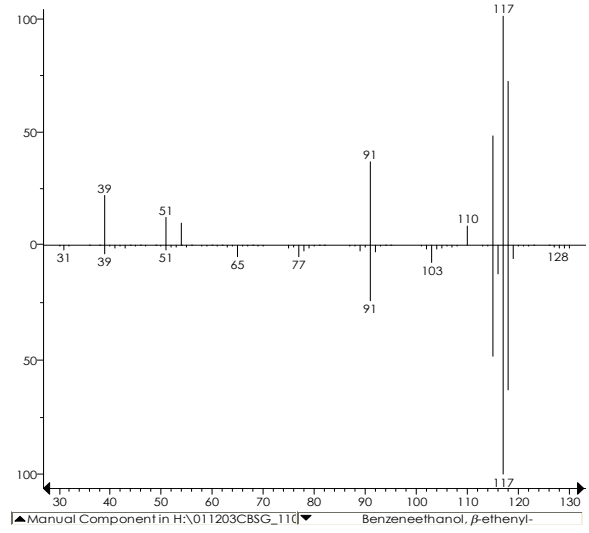
o-Methylstyrene (f.c. #105)



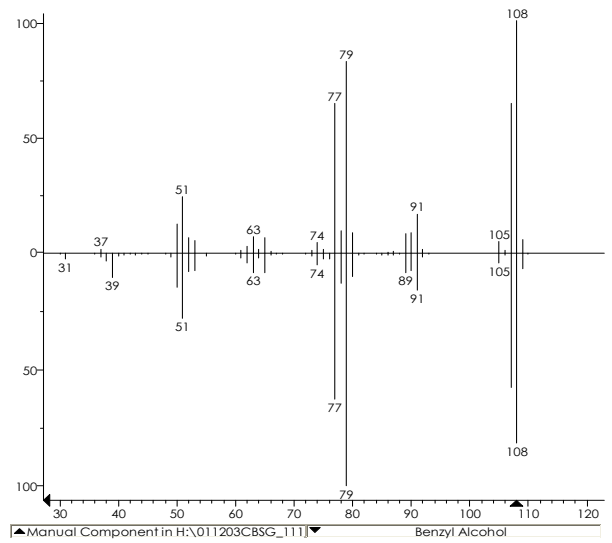
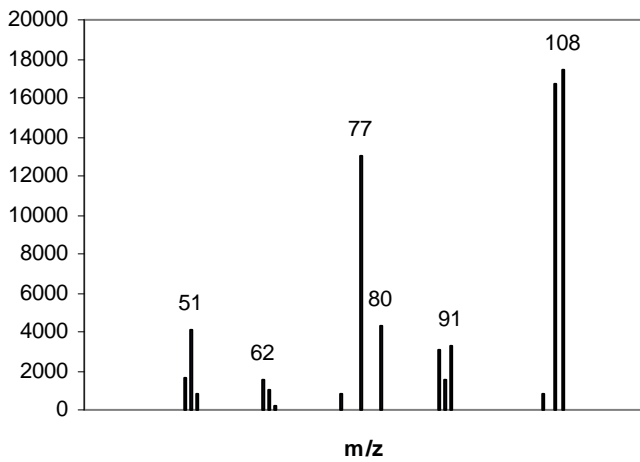
Benzonitrile (f. c. #104)



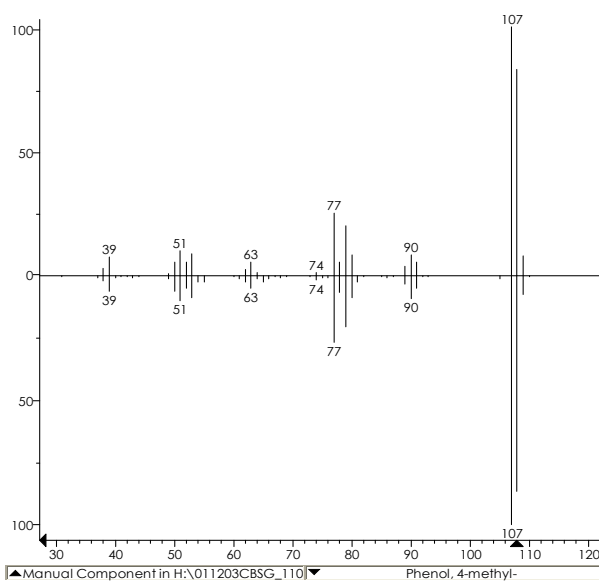
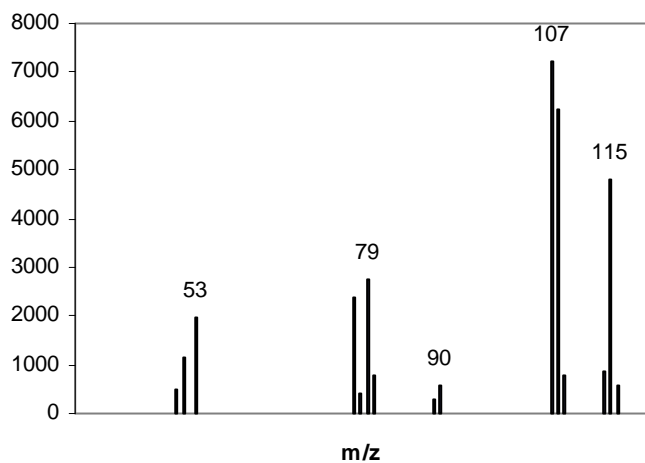
2-Phenyl-3-buten-1-ol (f.c. #156)



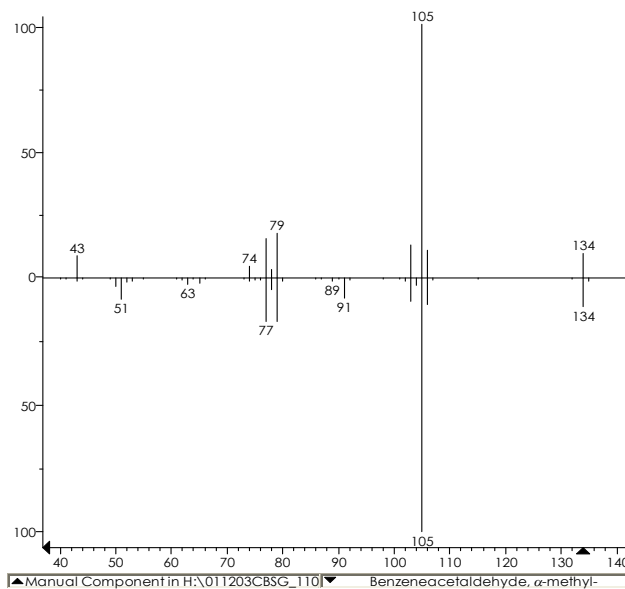
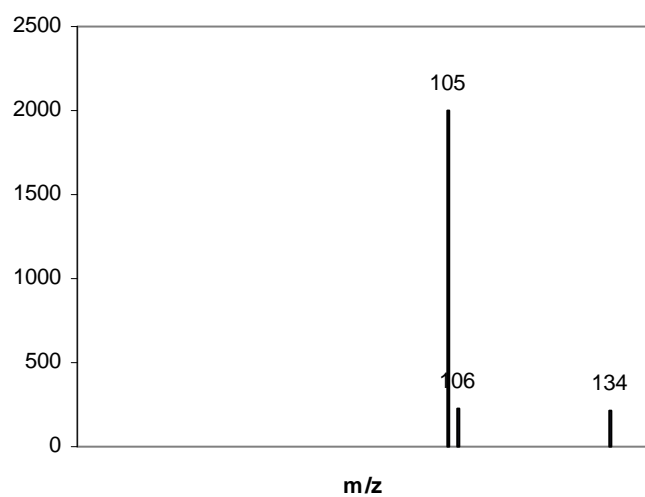
Benzyl alcohol (f.c. #125)



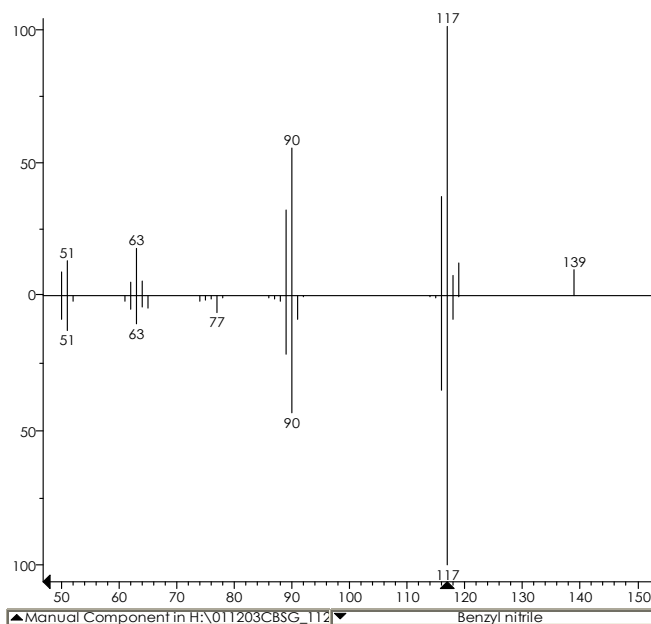
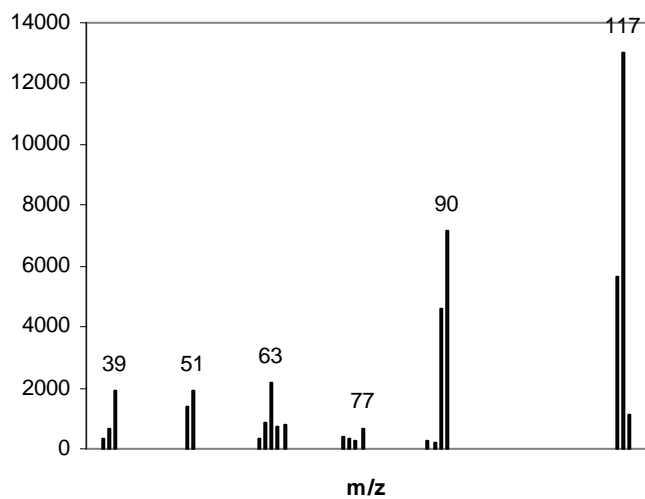
p-Cresol (f.c. #166)



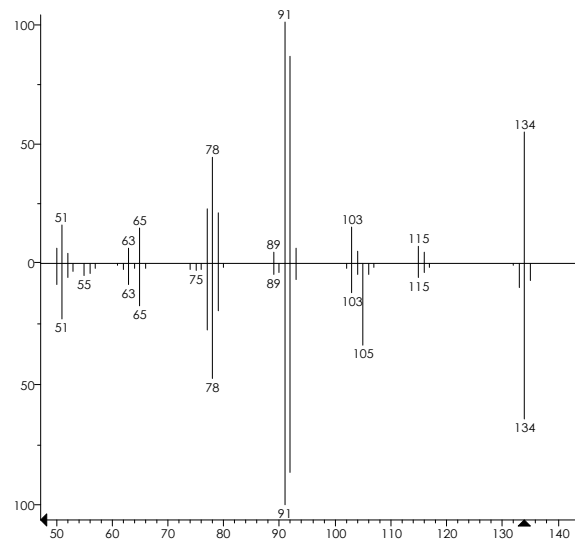
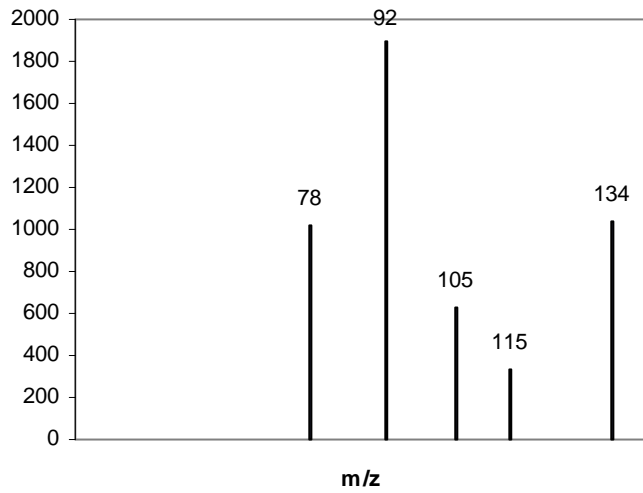
α -Phenylpropionaldehyde (f.c. #204)



Phenylacetonitrile (f.c. #202)

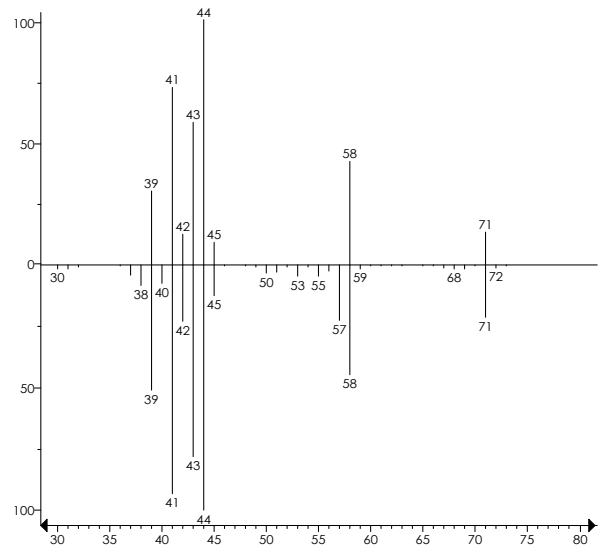
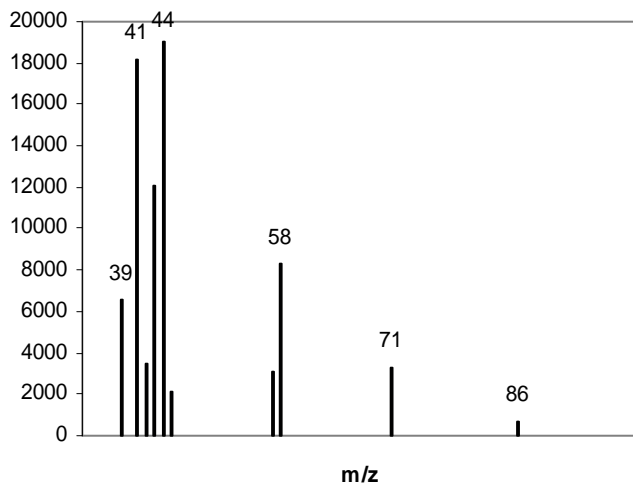


β -Phenylpropionaldehyde (f.c. #233)

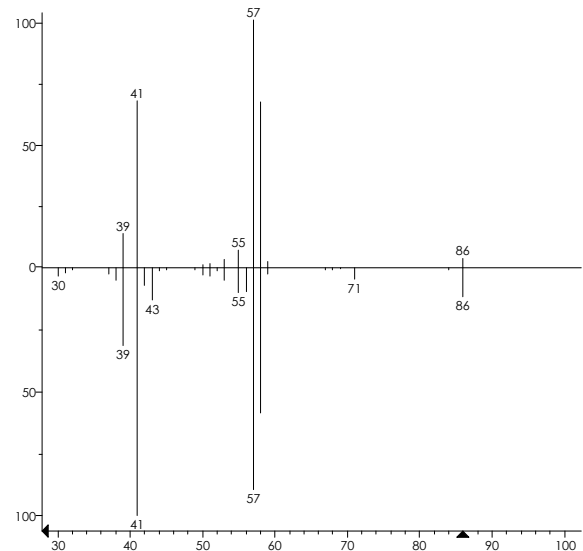
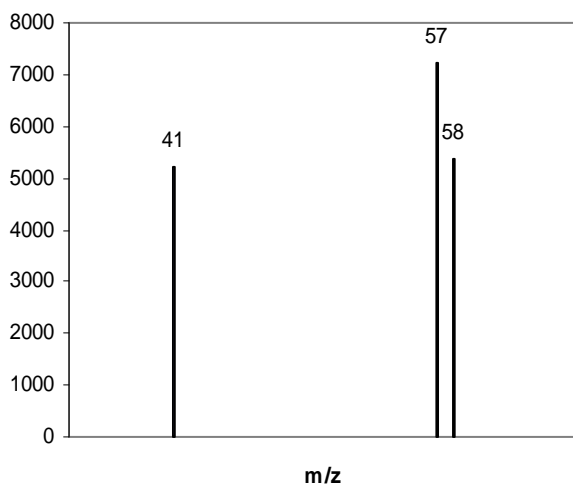


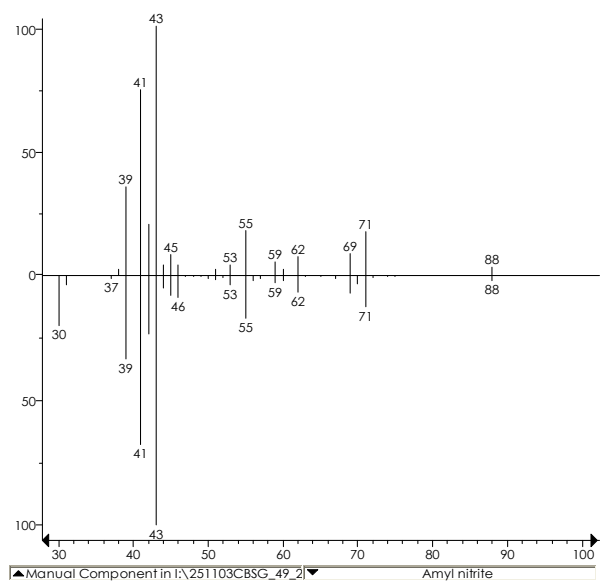
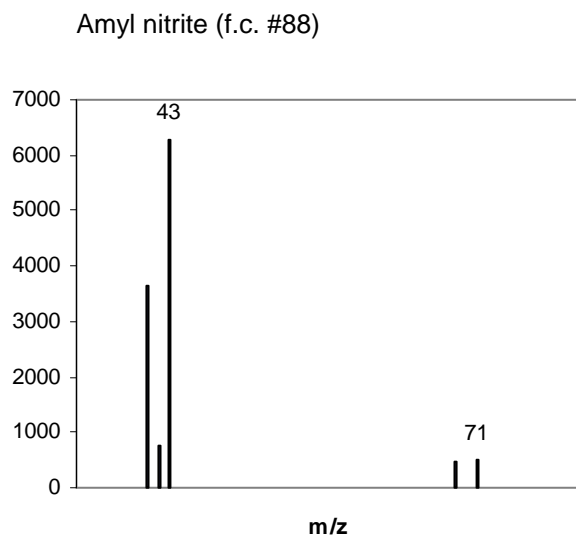
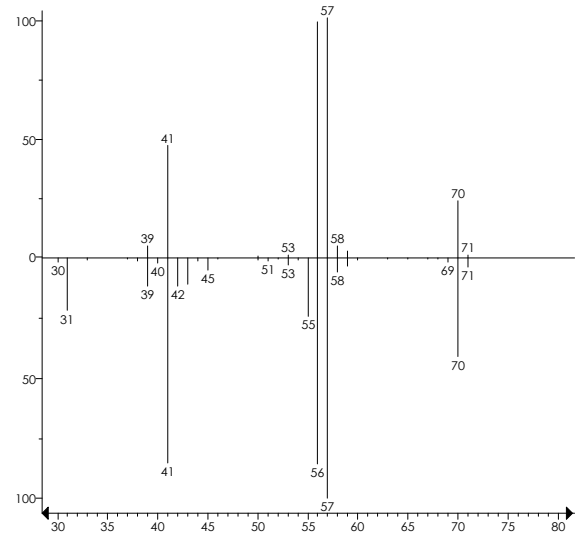
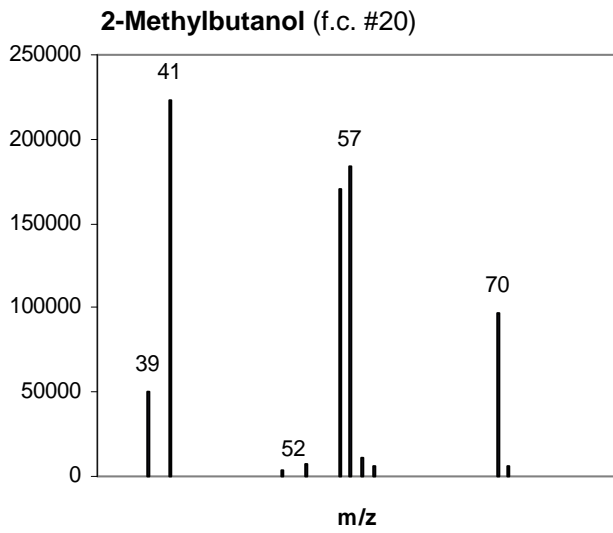
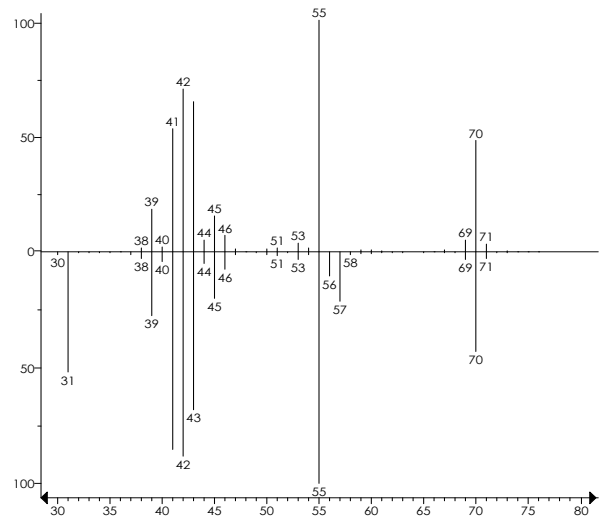
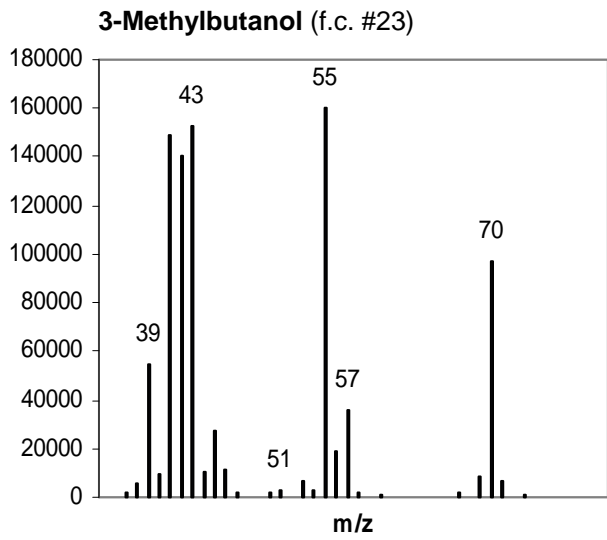
Leucine and Isoleucine derived volatiles

3-Methylbutanal (f.c. #22)

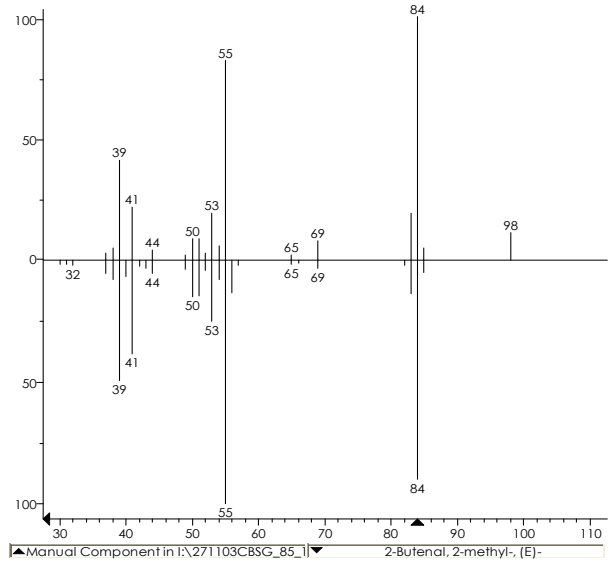
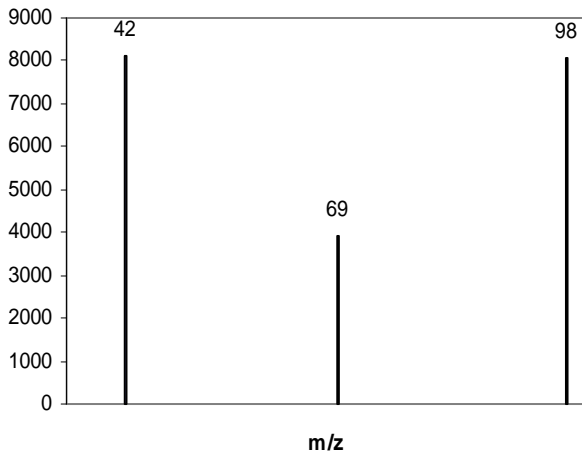


2-Methylbutanal (f.c. #19)

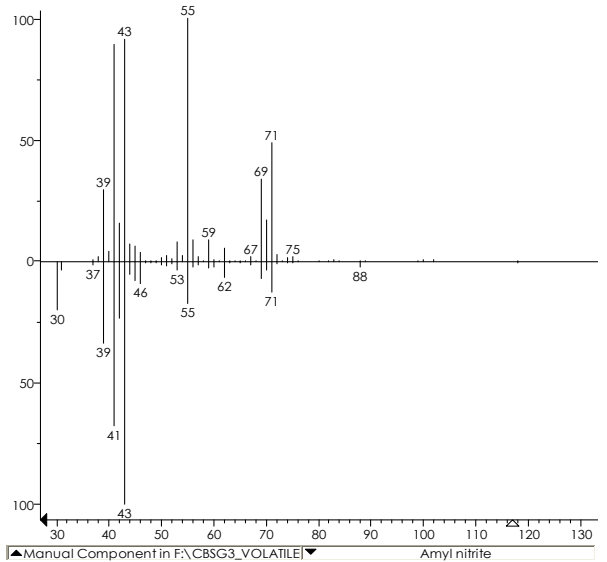
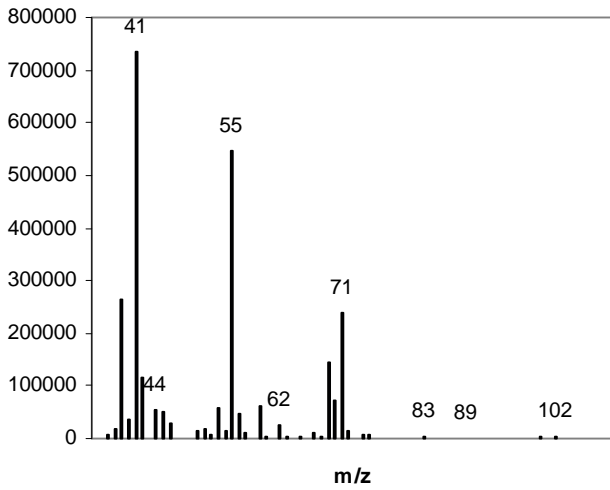




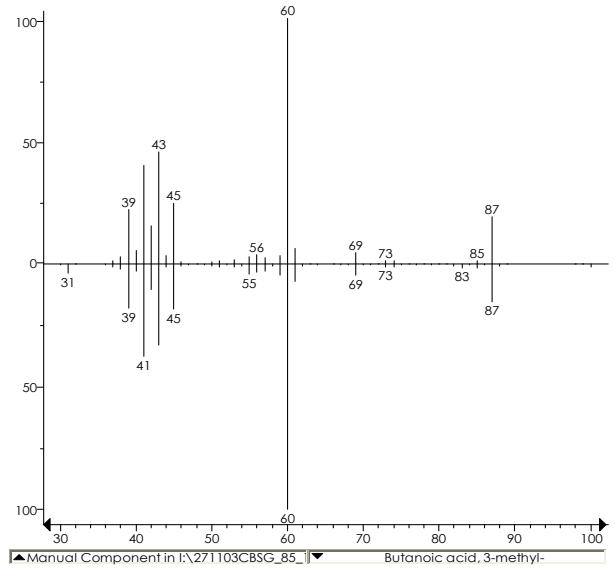
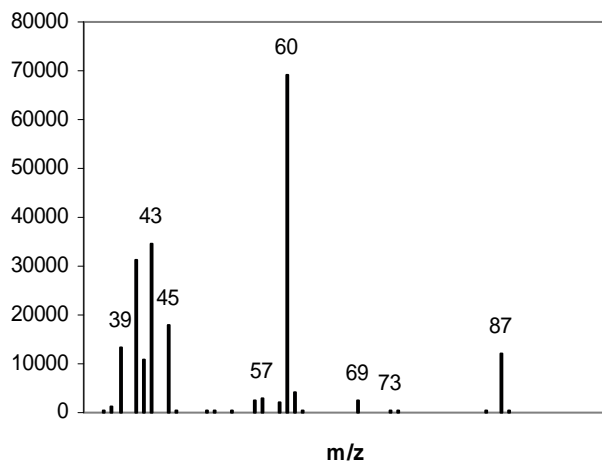
2-Butenal, 2-methyl-, (E)- (f.c. #45)



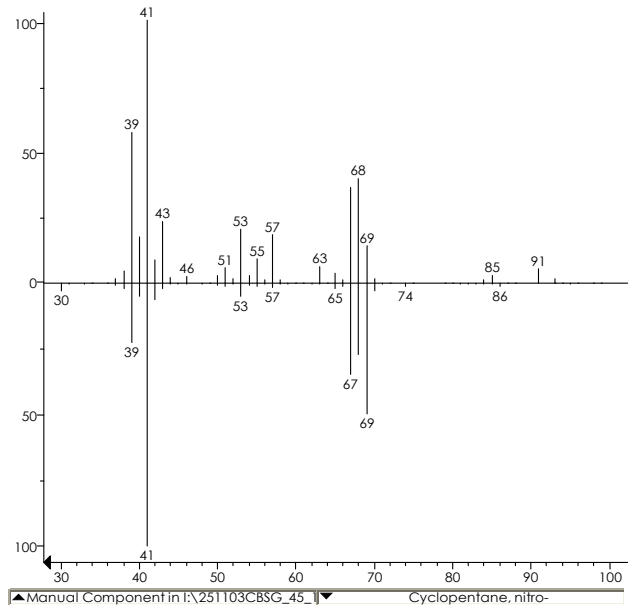
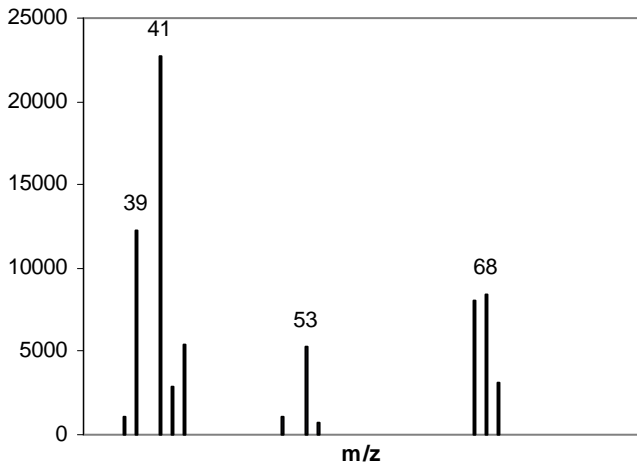
3-Methylbutanol nitrite (f.c. #80)



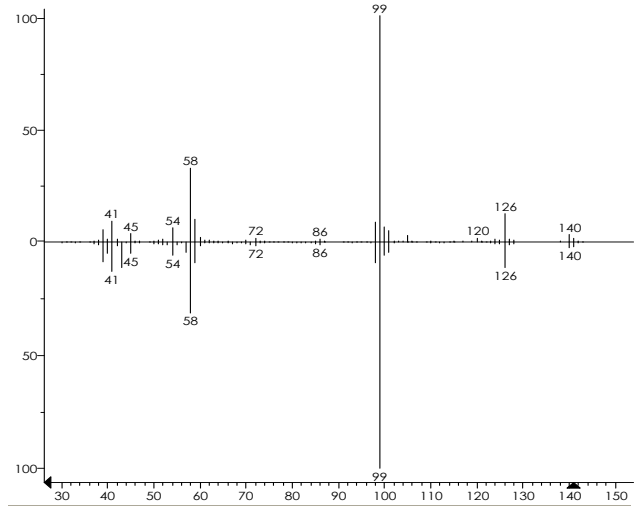
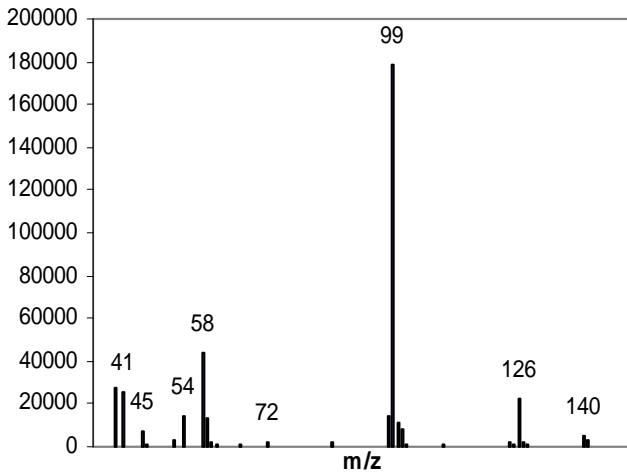
Butanoic acid, 3-methyl- (f.c. #29)



Nitrocyclopentane (f.c. #81)

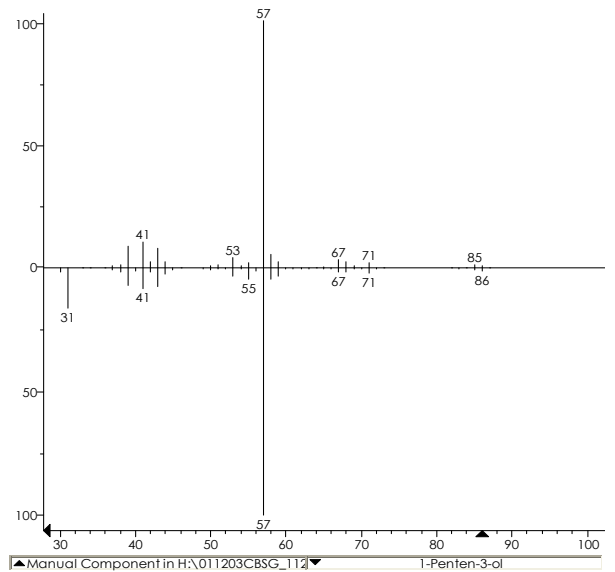
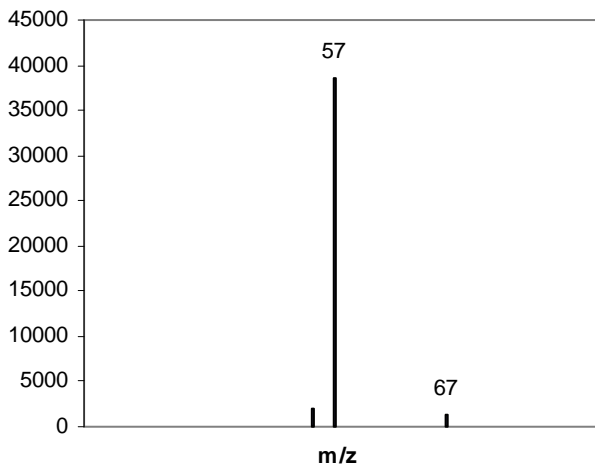


2-Isobutylthiazole (f.c. #162)

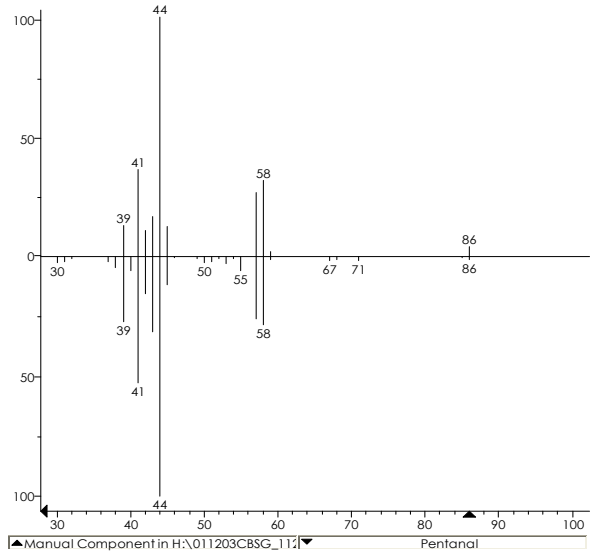
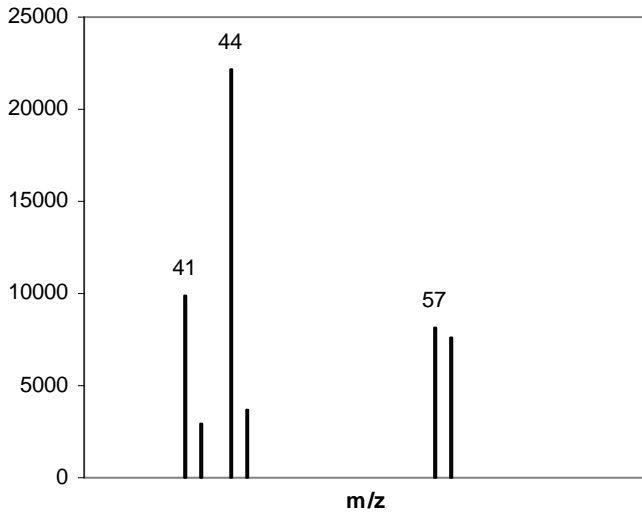


Lipid derived volatiles

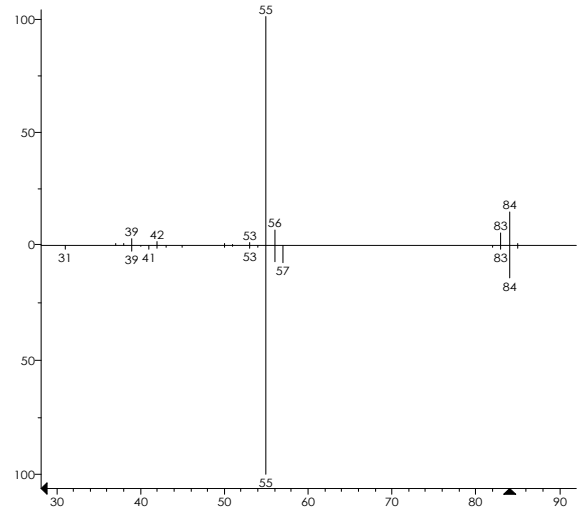
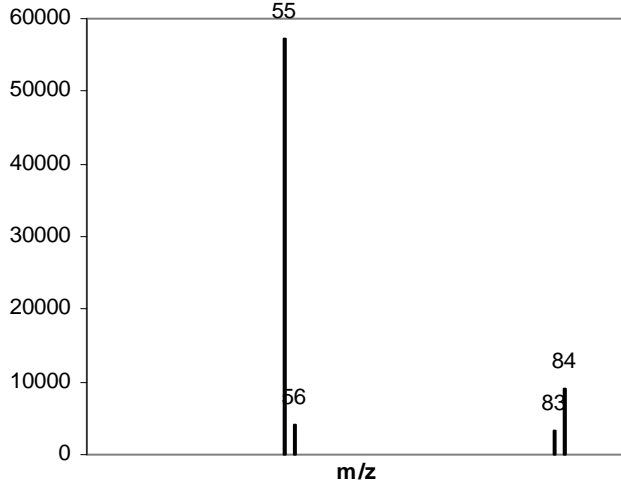
1-Penten-3-ol (f.c. #15)



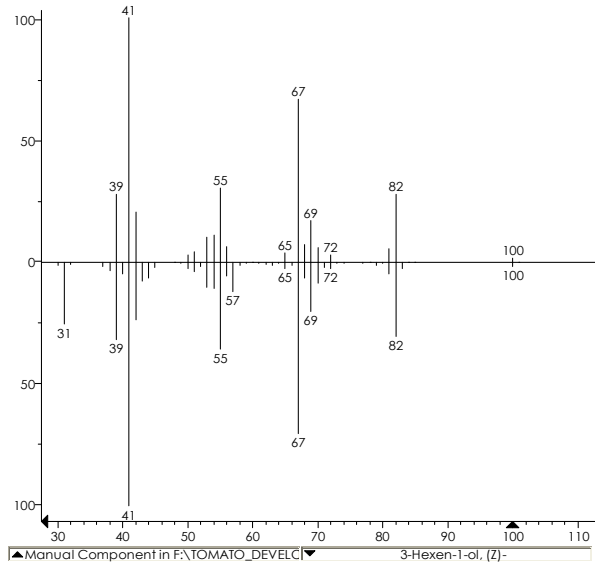
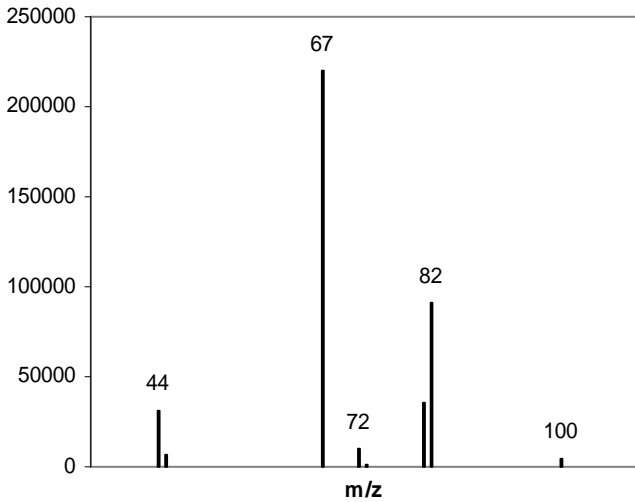
Pentanal (f.c. #10)

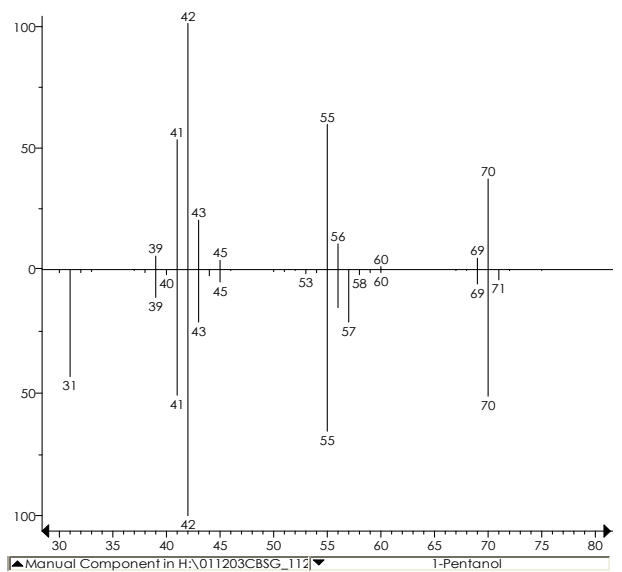
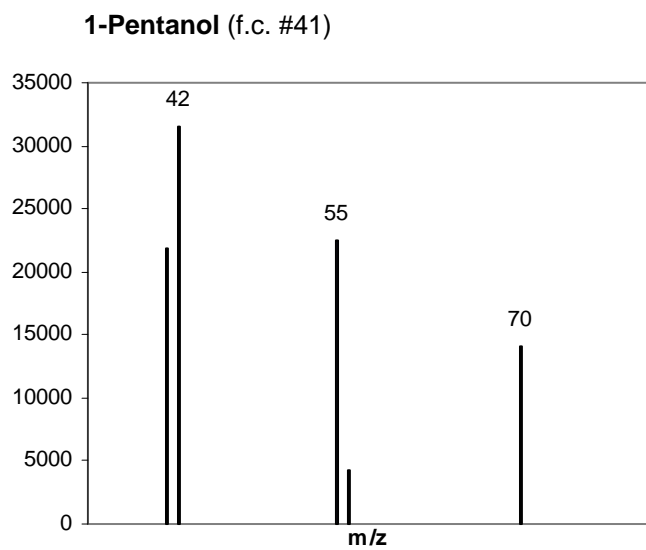
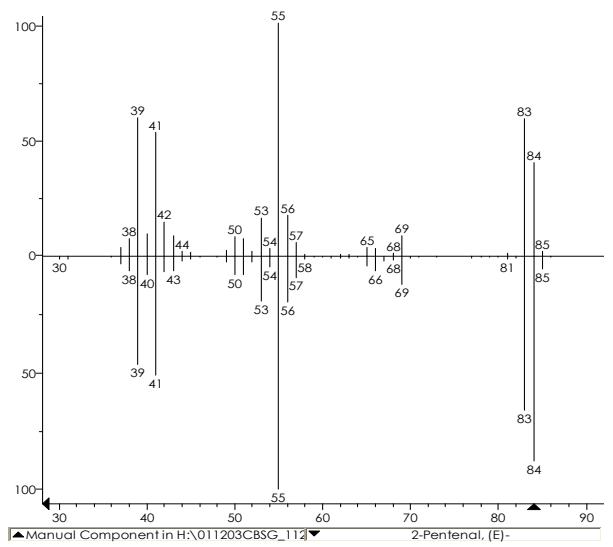
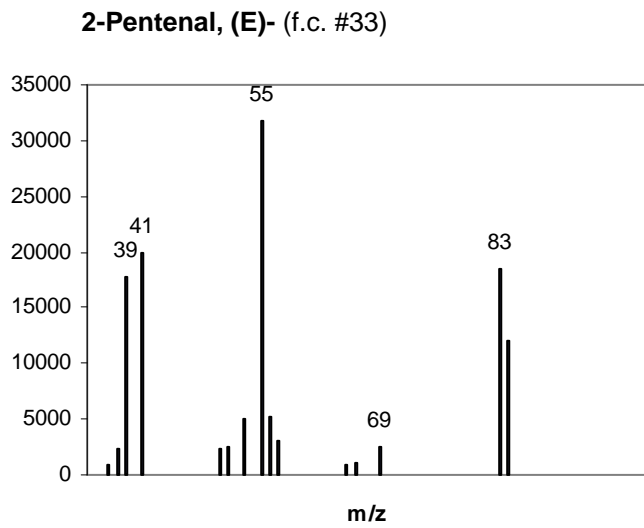
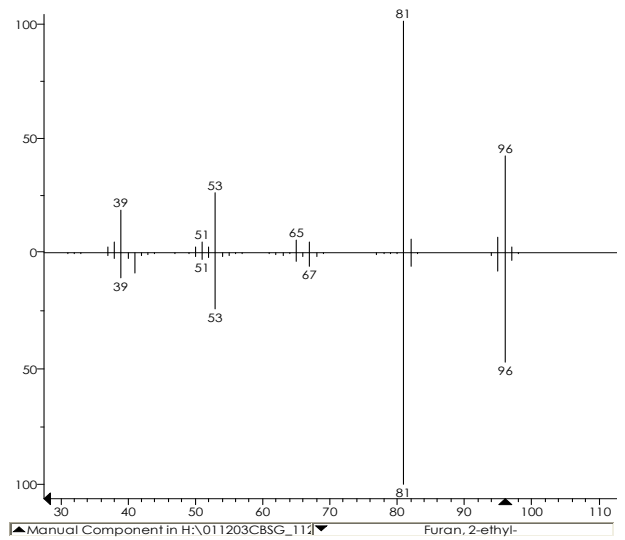
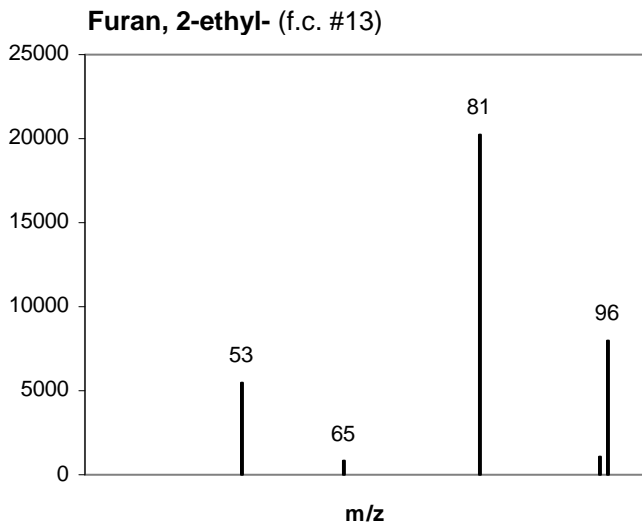


1-Penten-3-one (f.c. #16)

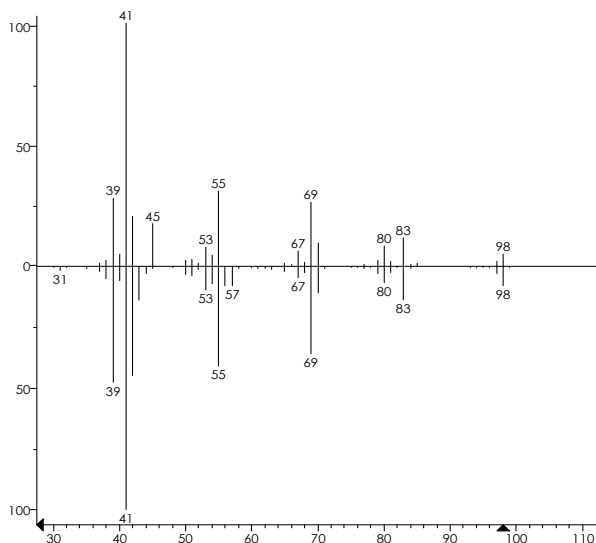
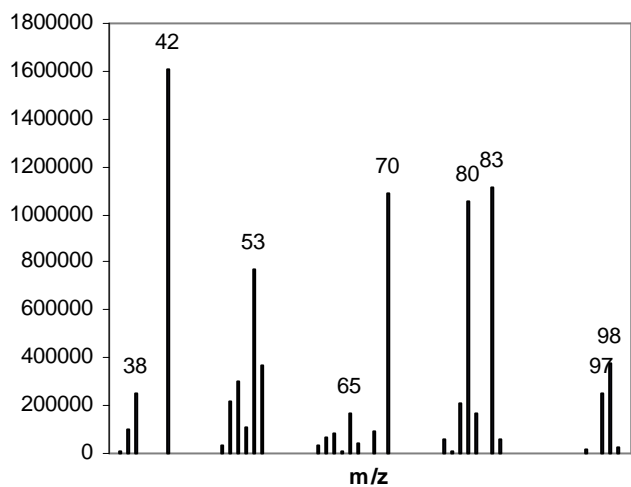


Z-3-Hexenol (f.c. #49)

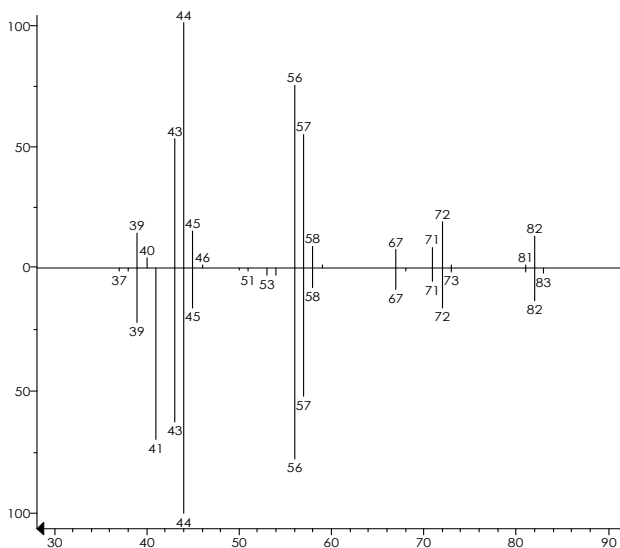
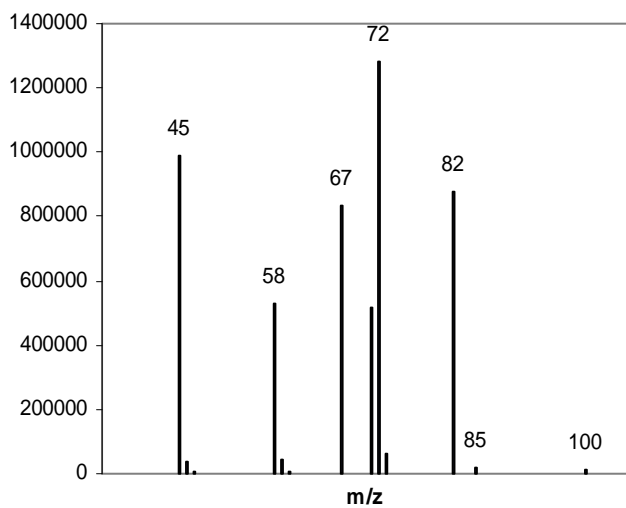




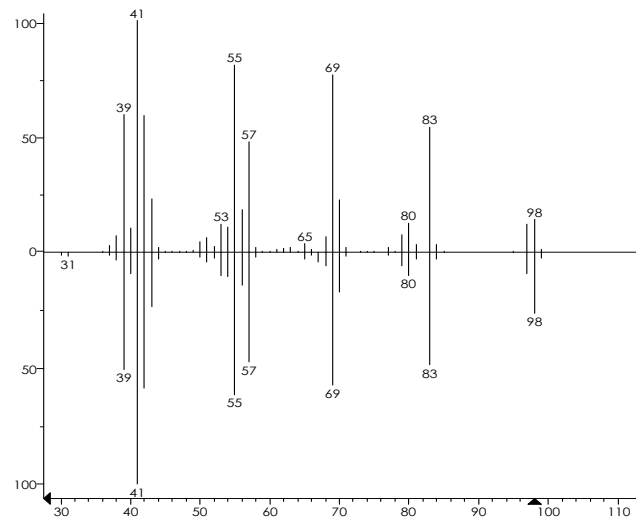
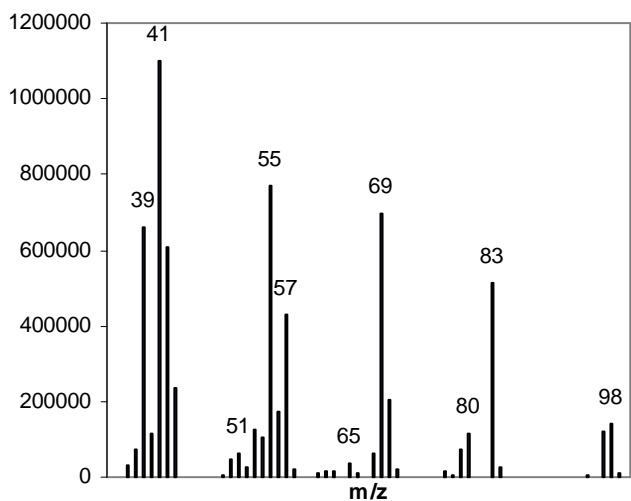
Z-3-Hexenal (f.c. #37)



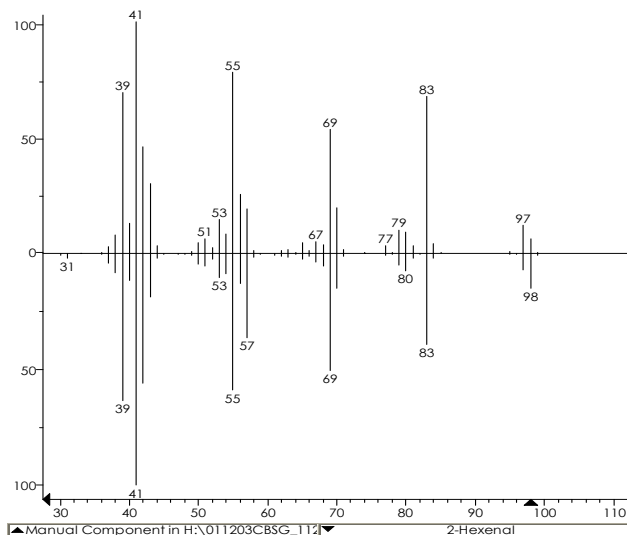
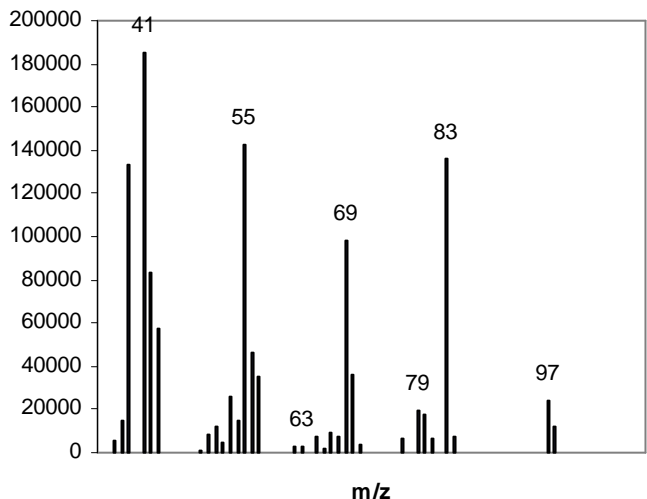
Hexanal (f.c. #39)



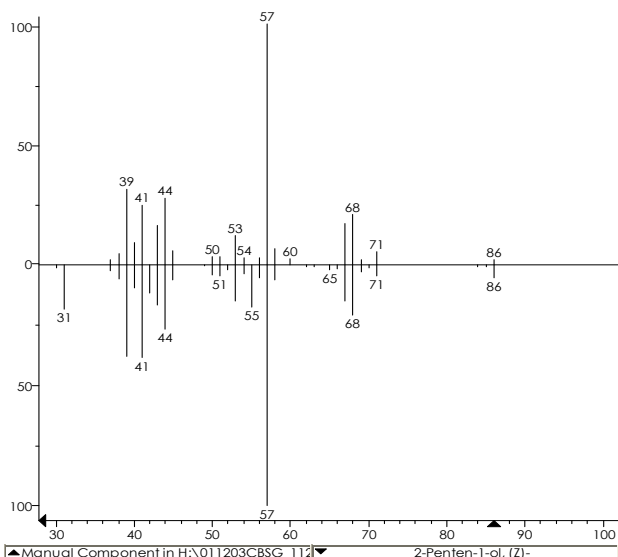
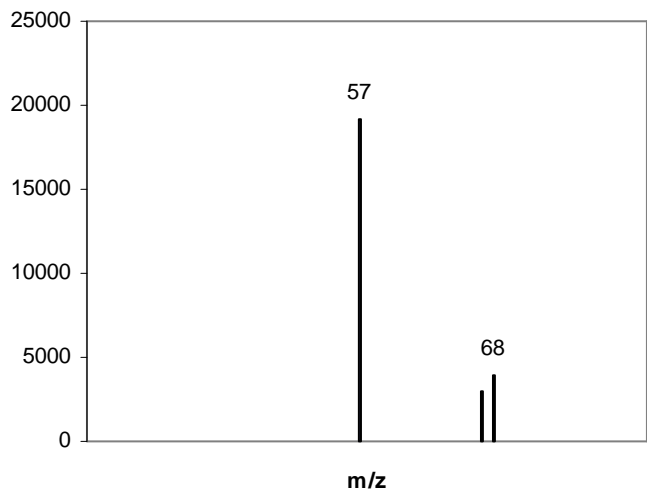
E-2-Hexenal (f.c. #57)



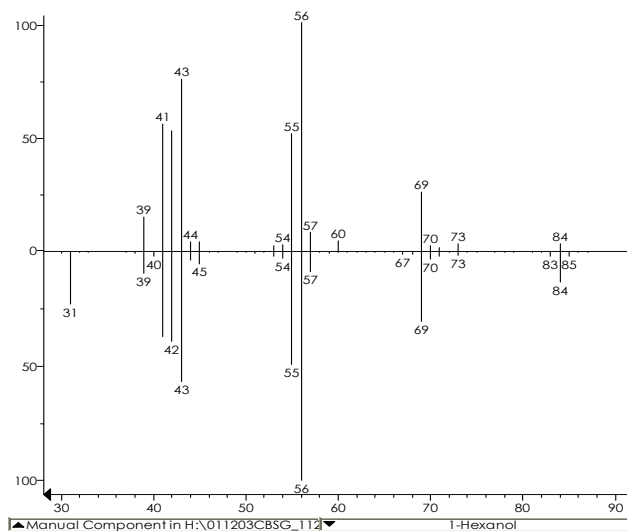
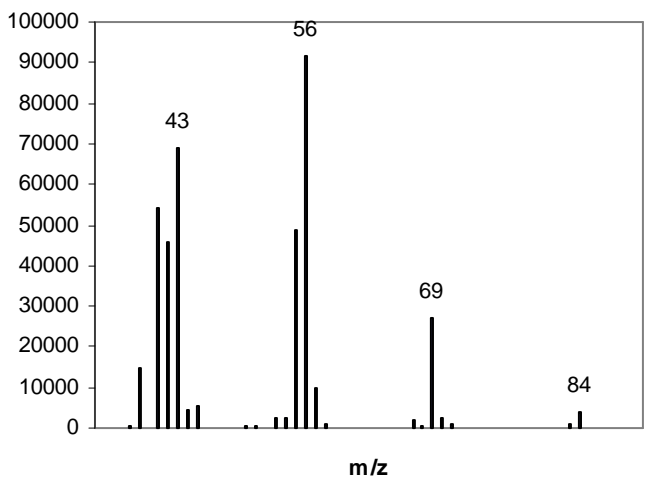
2-Hexenal (f.c. #55)



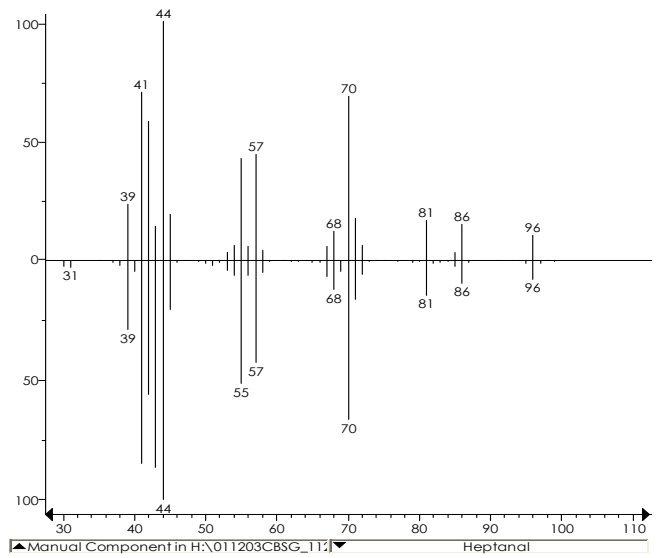
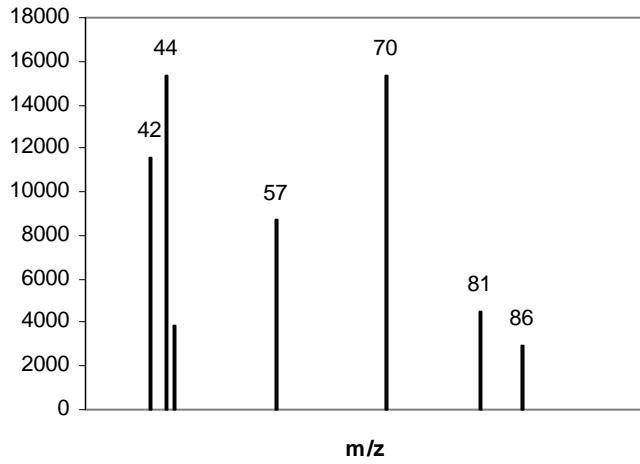
Z-2-Penten-1-ol (f.c. #47)



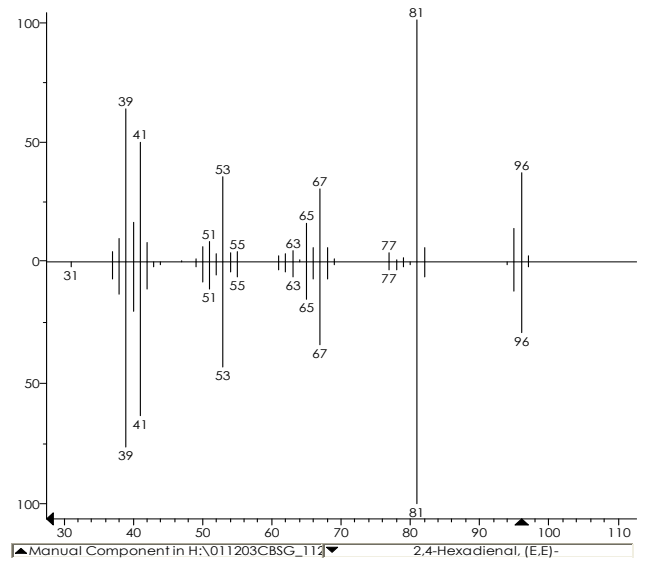
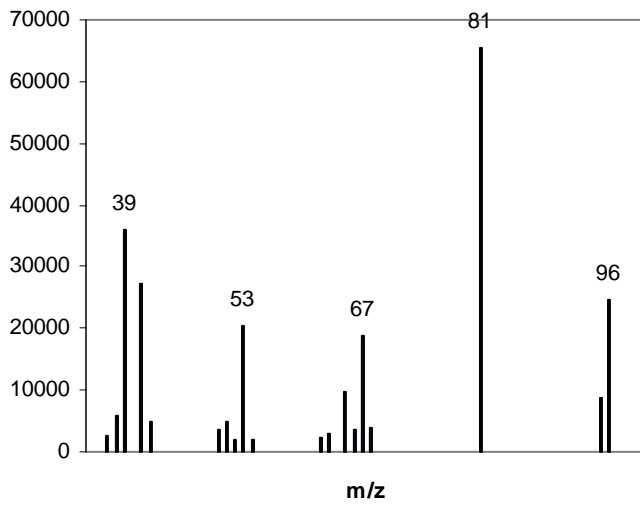
1-Hexanol (f.c. #71)



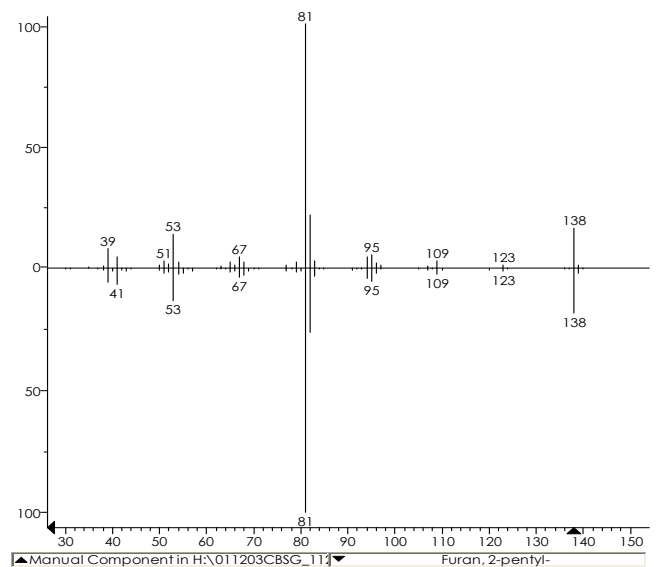
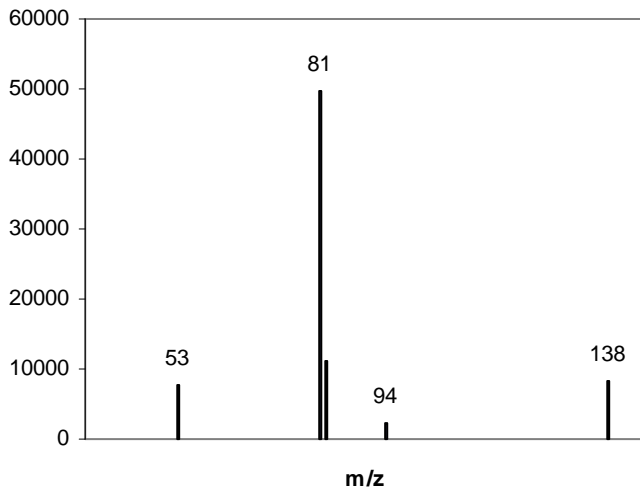
Heptanal (f.c. #99)



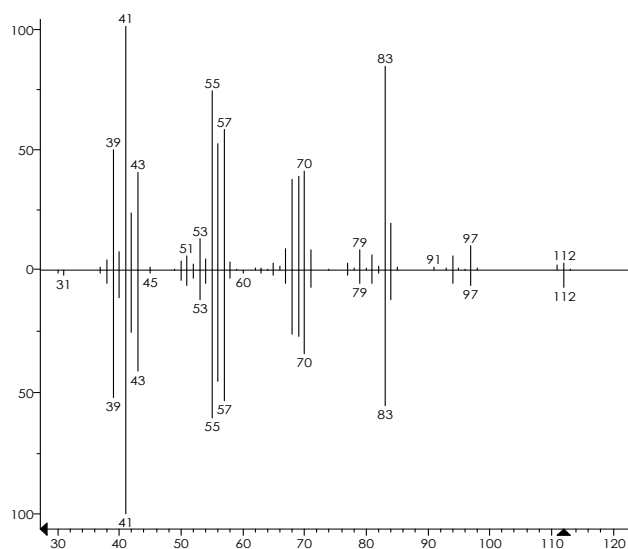
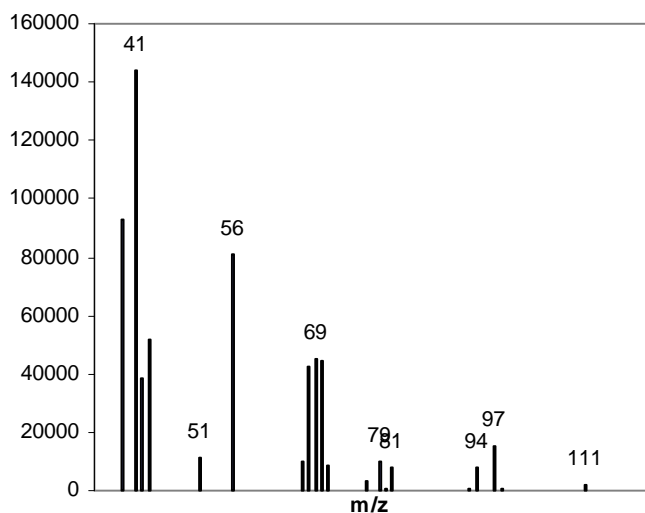
E,E-2,4-Hexadienal (f.c. #94)



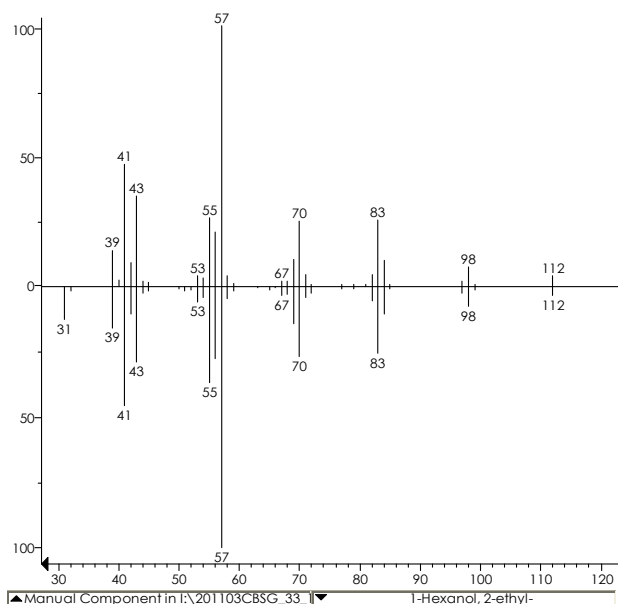
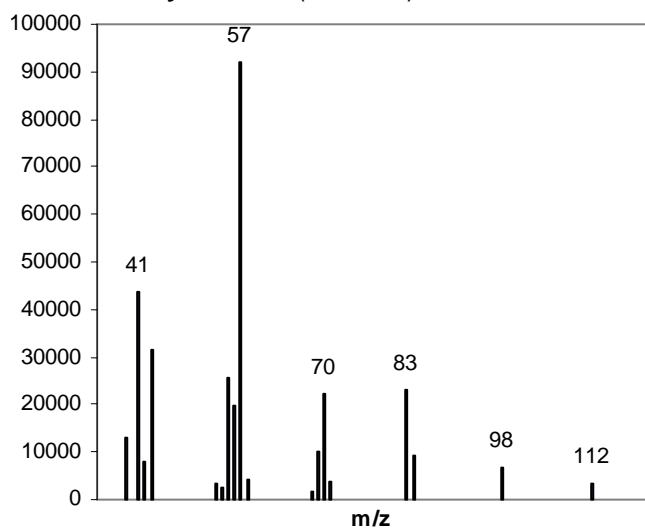
2-Pentylfuran (f.c. #112)



E-2-Heptenal (f.c. #92)

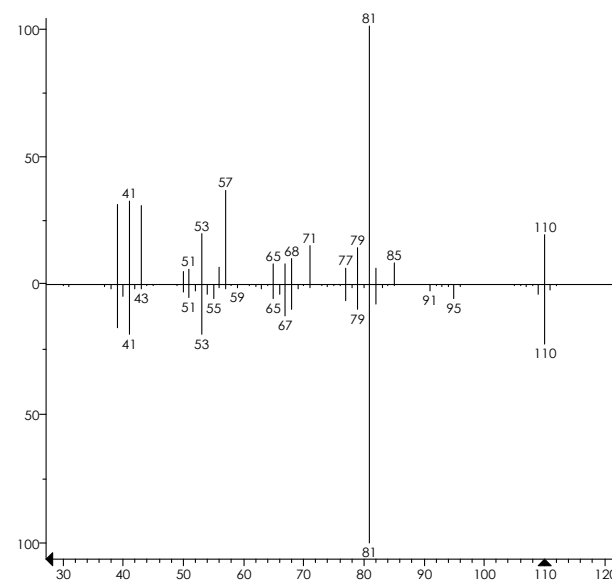
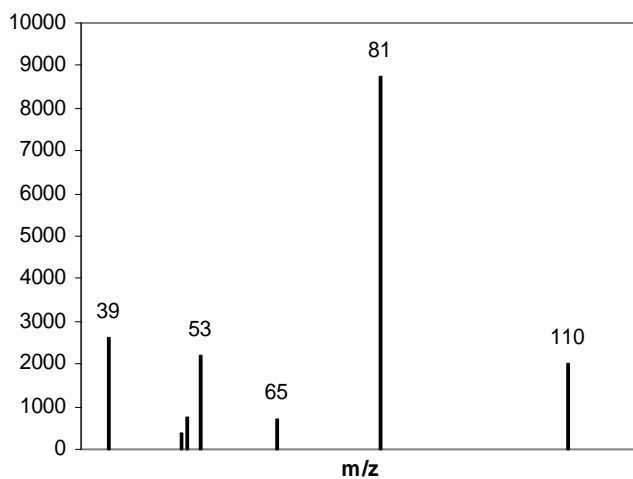


2-Ethylhexanol (f.c. #150)



Manual Component in I:\201103CBSG_33_1 1-Hexanol, 2-ethyl-

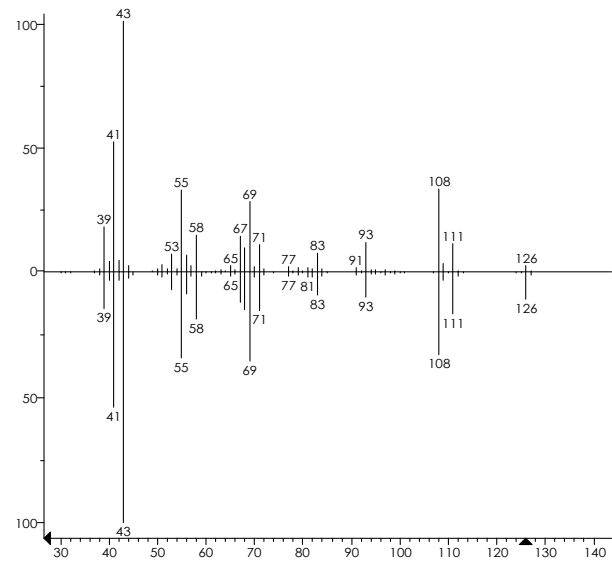
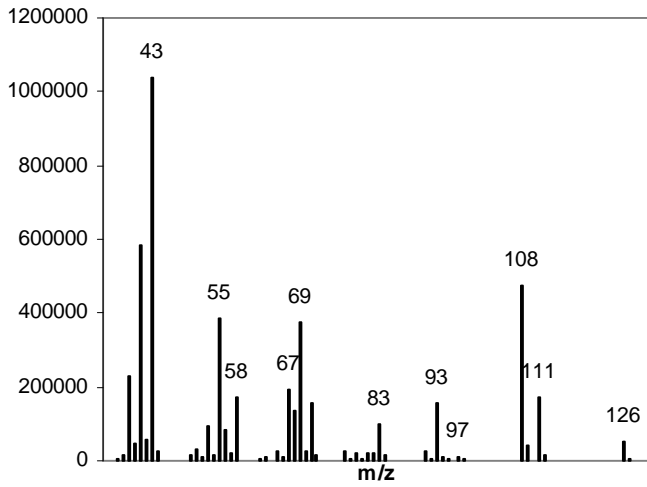
E,E-2,4-Heptadienal (f.c. #109)



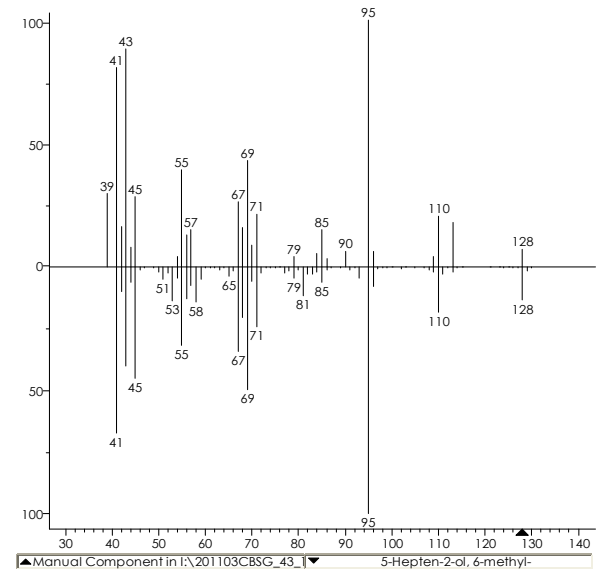
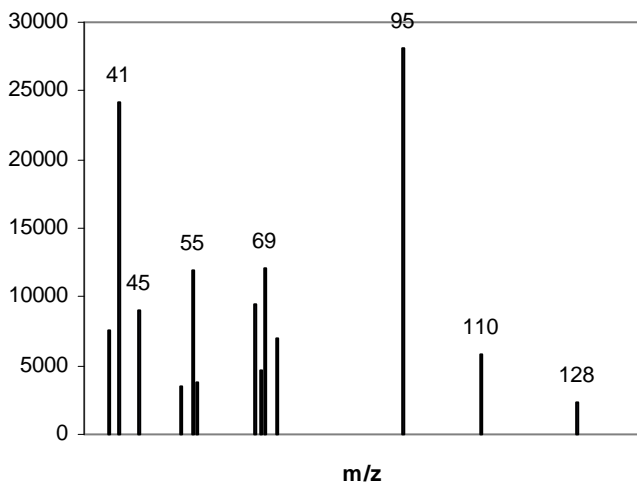
Manual Component in I:\201103CBSG_33_1 2,4-Heptadienal, (E,E)-

Open chain carotenoid derivatives

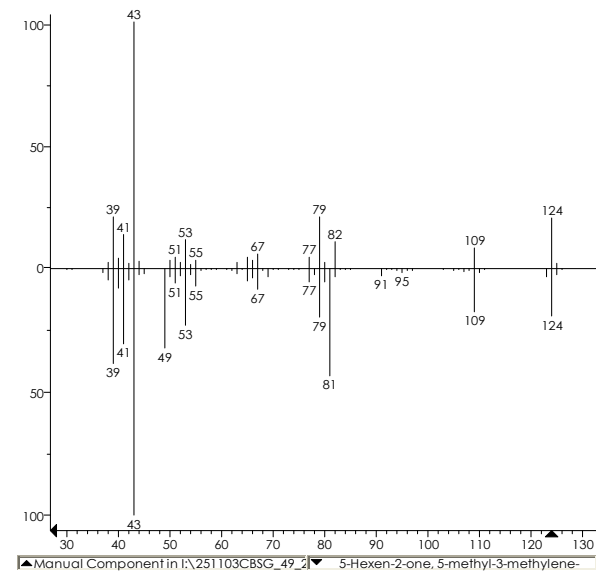
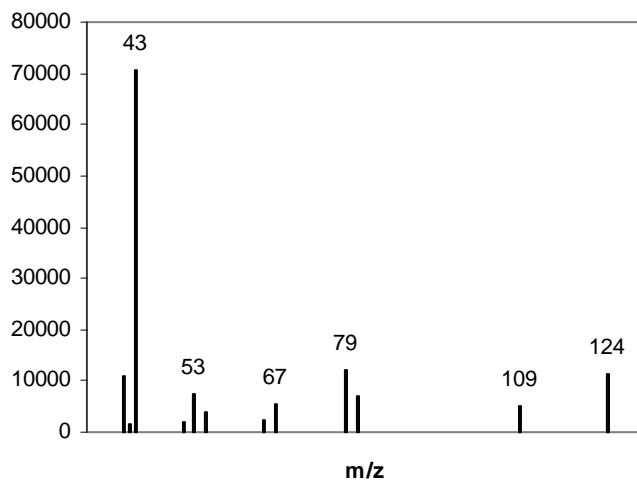
6-Methyl-5-hepten-2-one (f.c. #120)



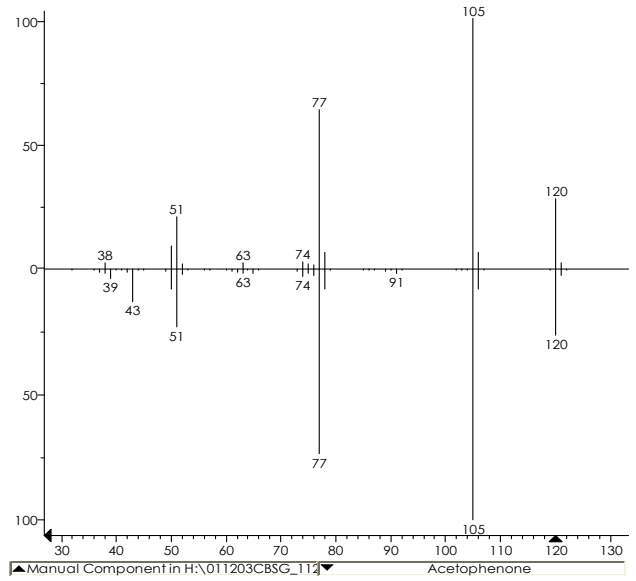
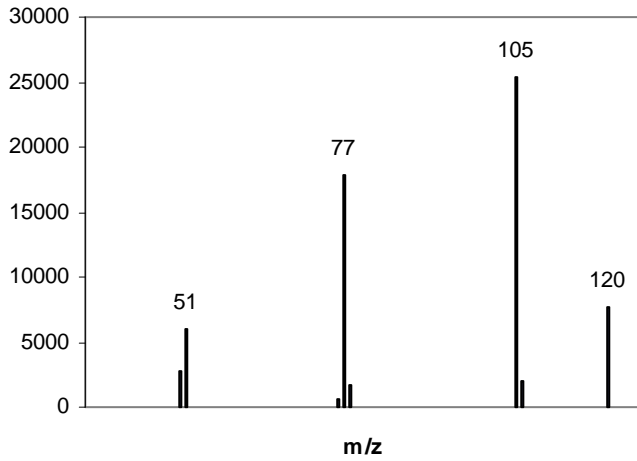
5-Hepten-2-ol, 6-methyl- (f.c. #118)



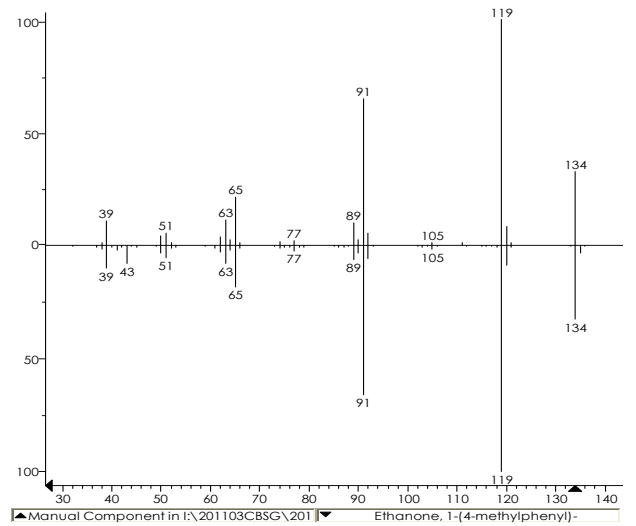
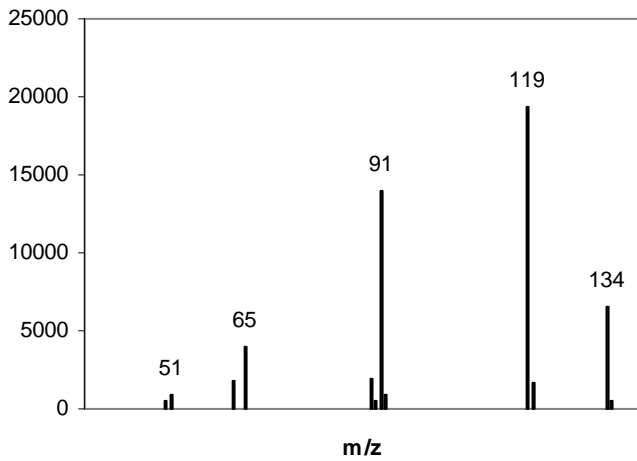
5-Hexen-2-one, 5-methyl-3-methylene- (f.c. #161)



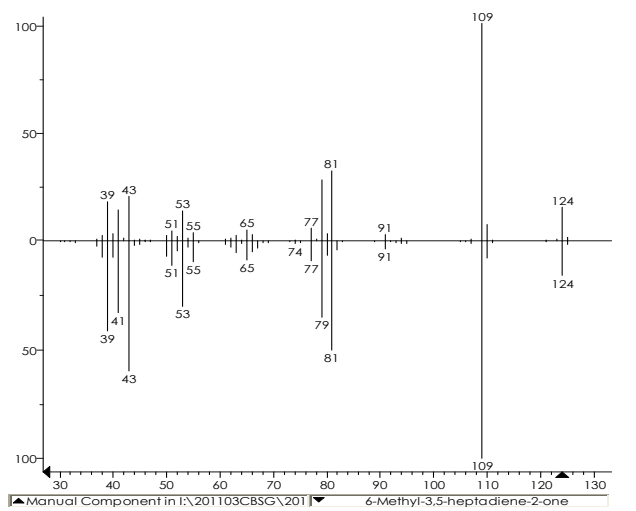
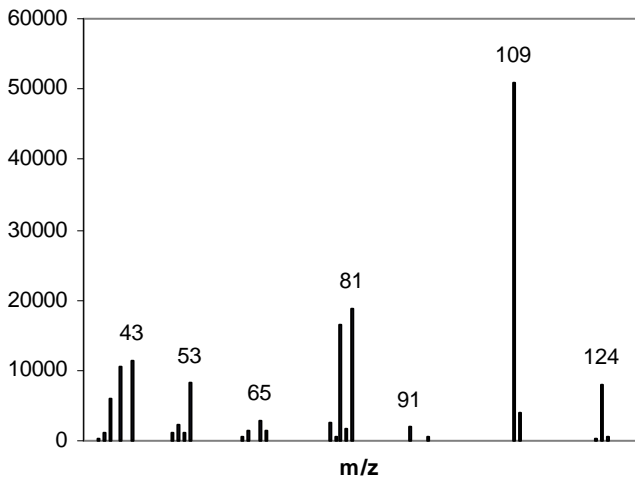
Acetophenone (f.c. #183)

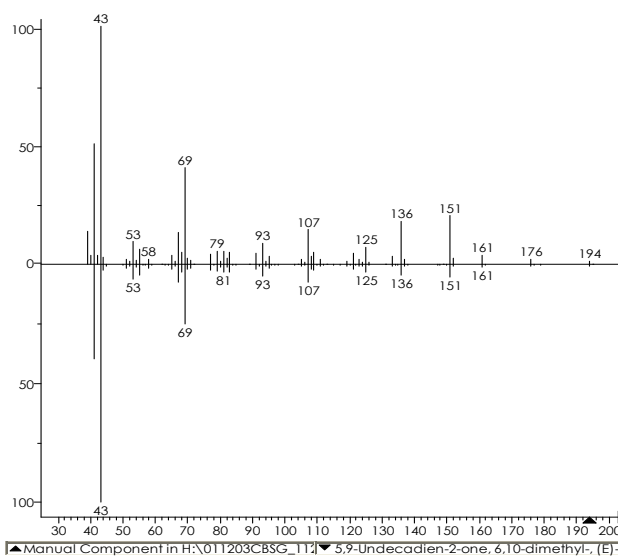
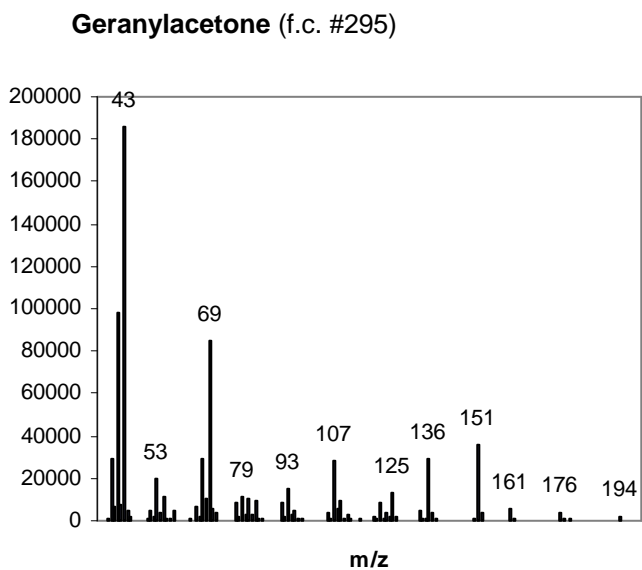
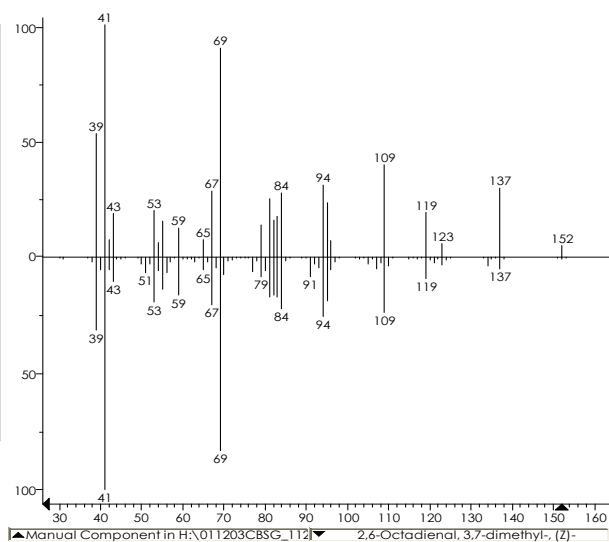
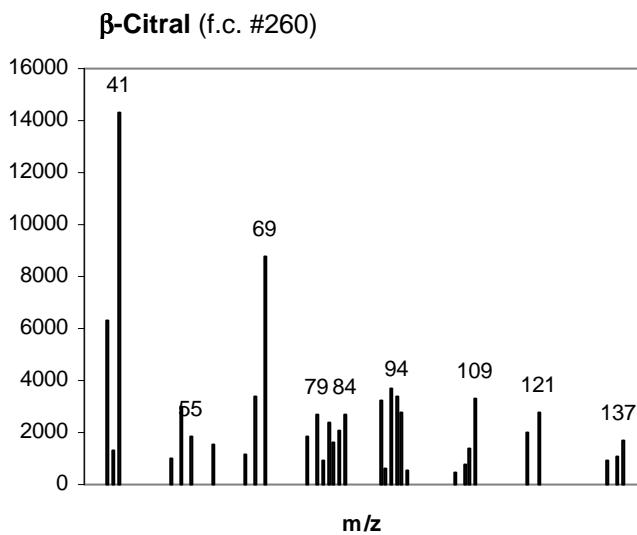
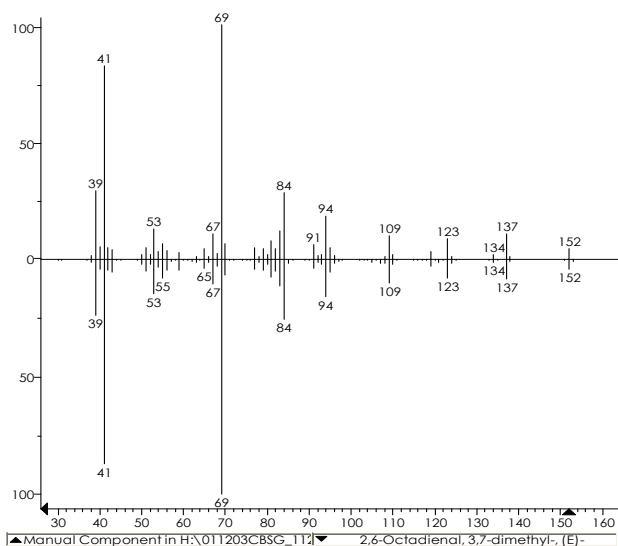
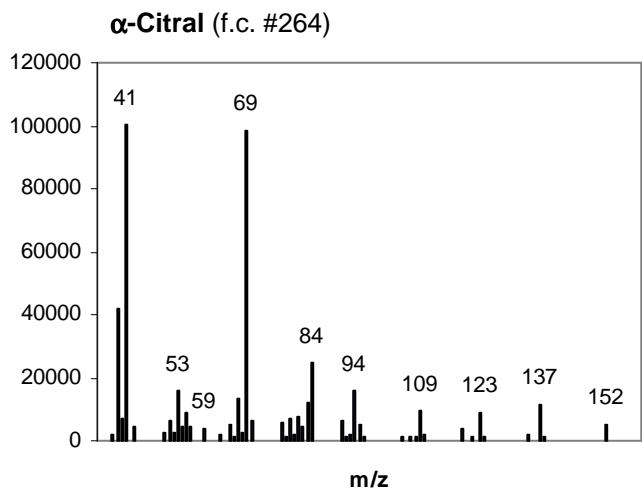


4'-Methylacetophenone (f.c. #238)

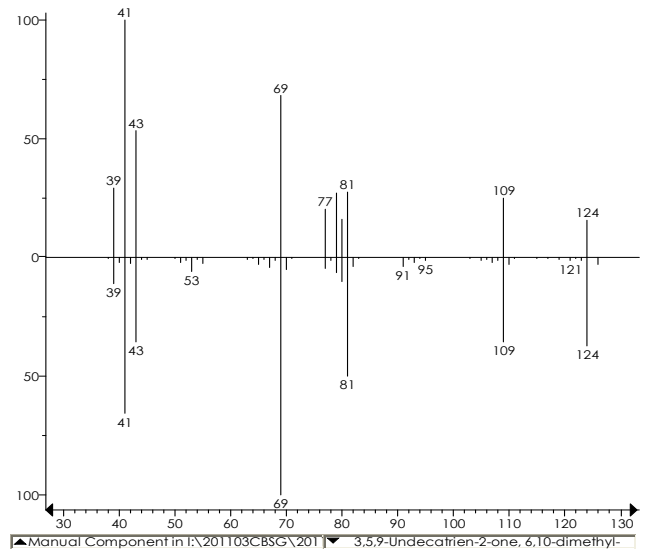
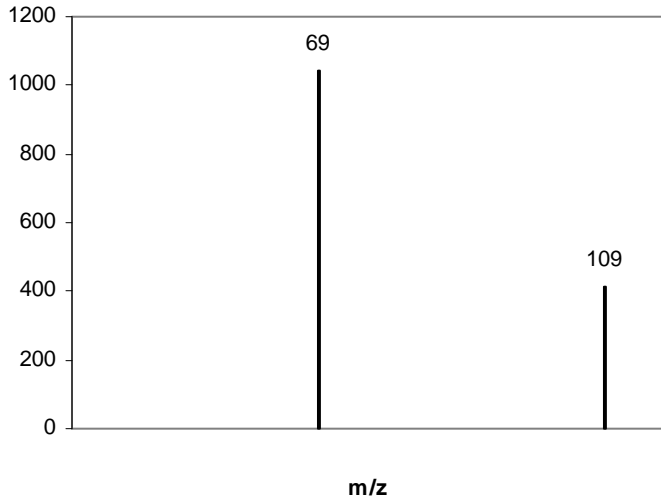


6-Methyl-3,5-heptadiene-2-one (f.c. #216)



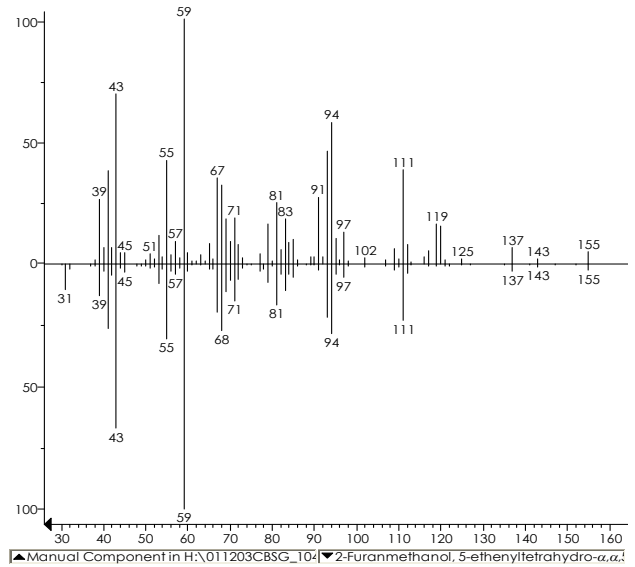
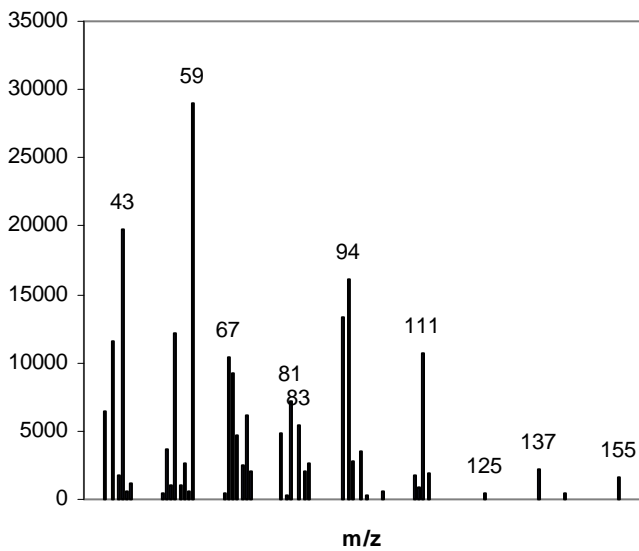


Pseudoionone (f.c. #303)

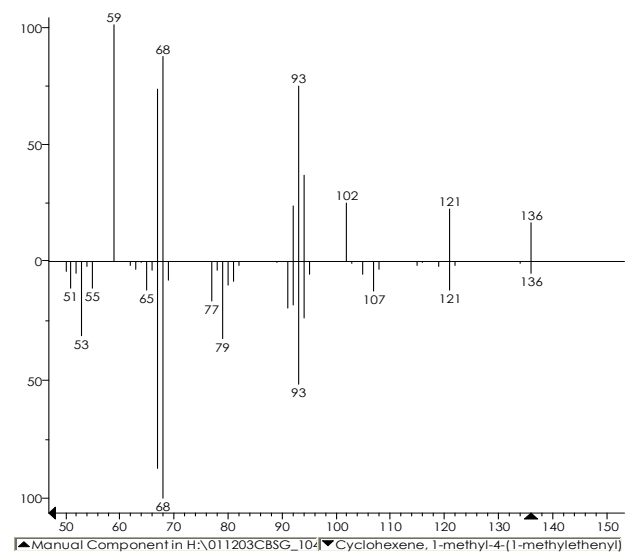
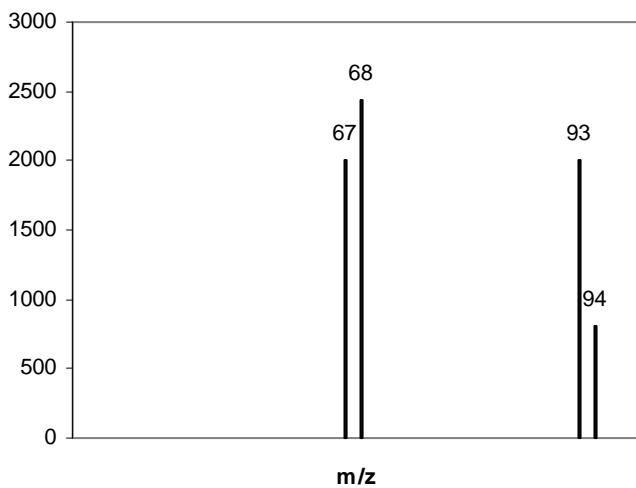


Terpenoids

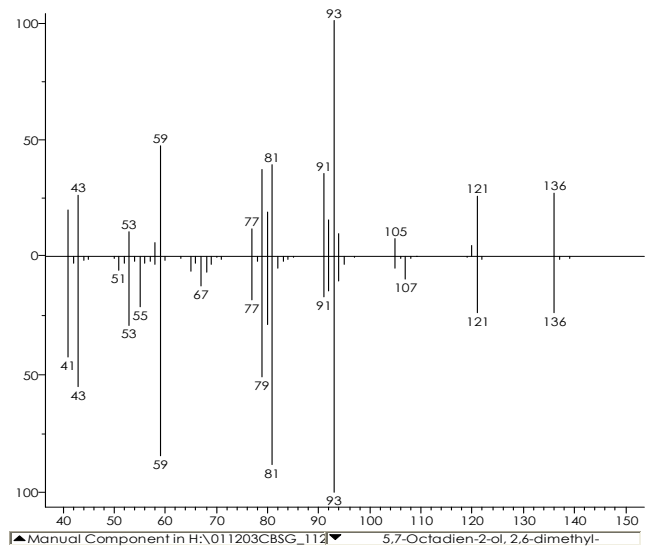
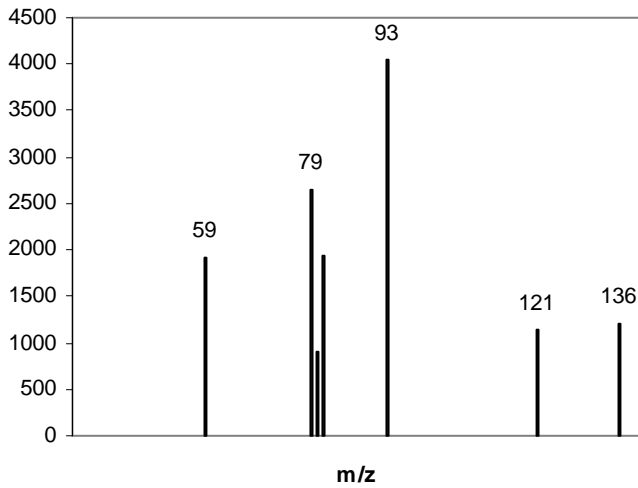
Z-Linalool oxide (f.c. 142)



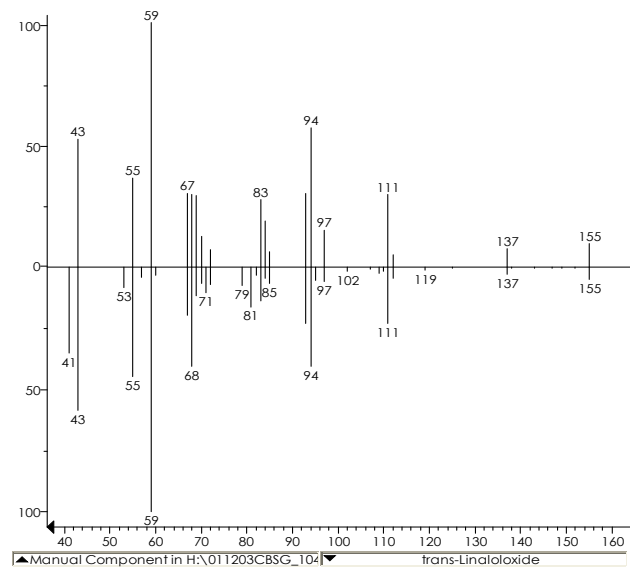
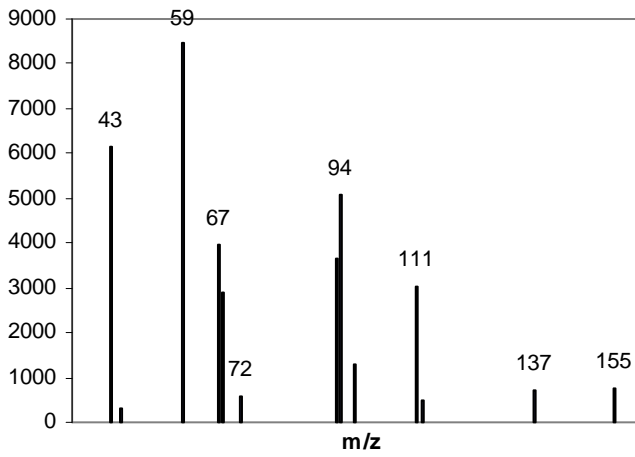
Limonene (f.c. #142)



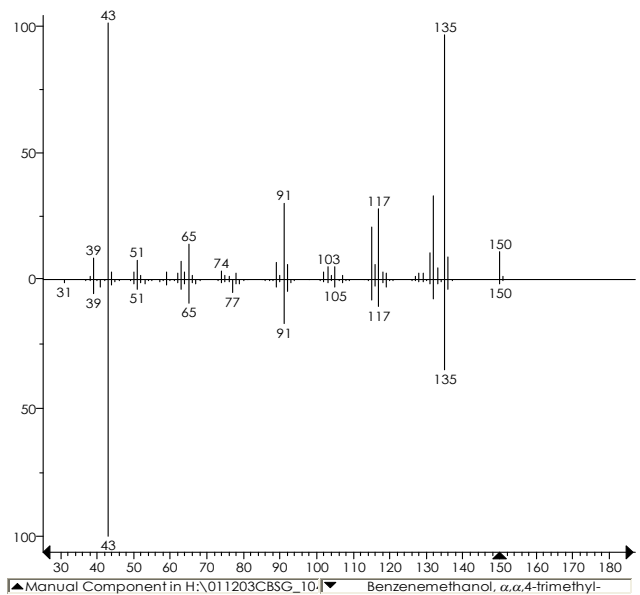
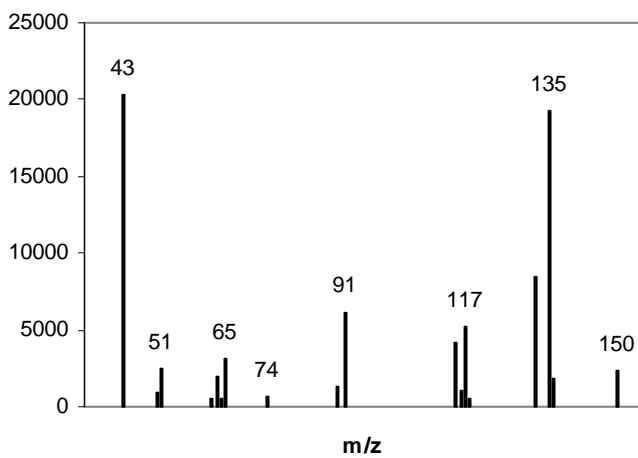
Ocimenol (f.c. #212)



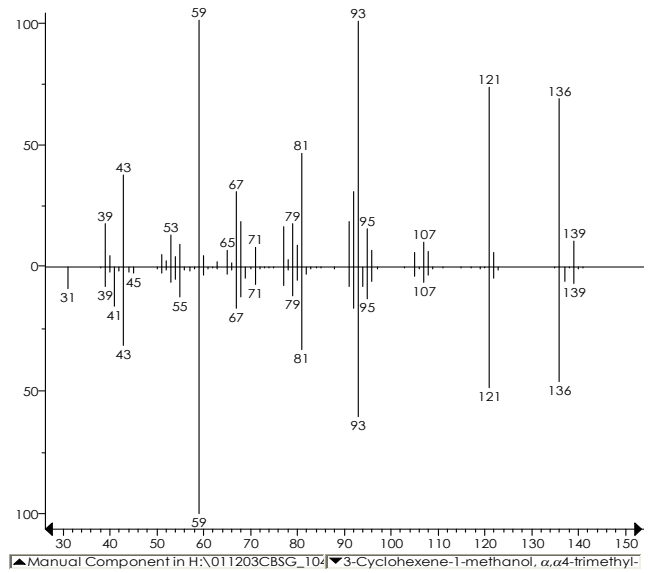
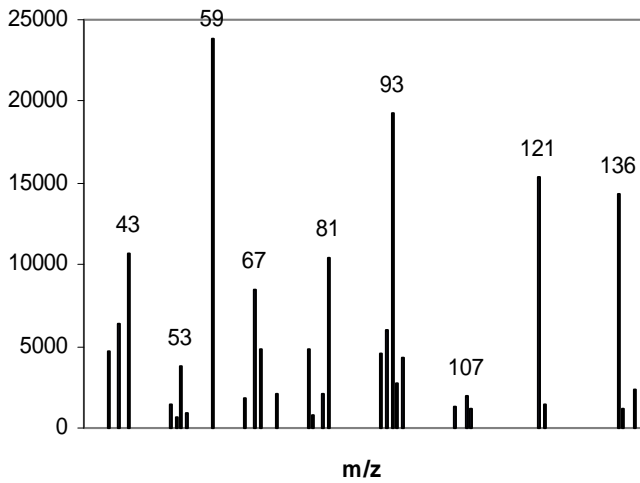
E-Linalool oxide (f.c. #174)



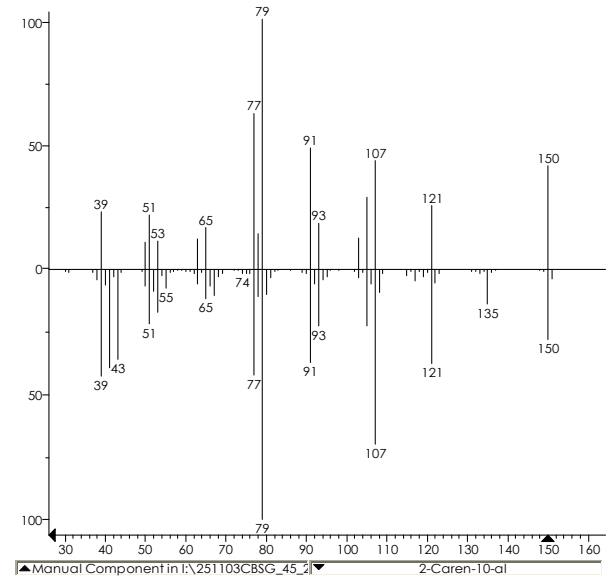
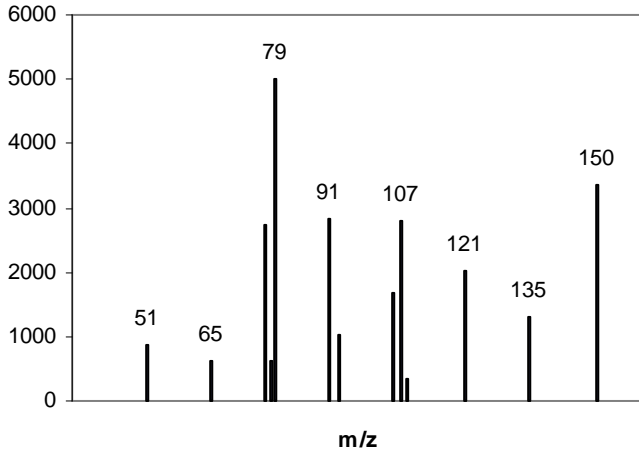
p-Cimanol-8-ol (f.c. #239)



α -Terpineol (f.c. #240)

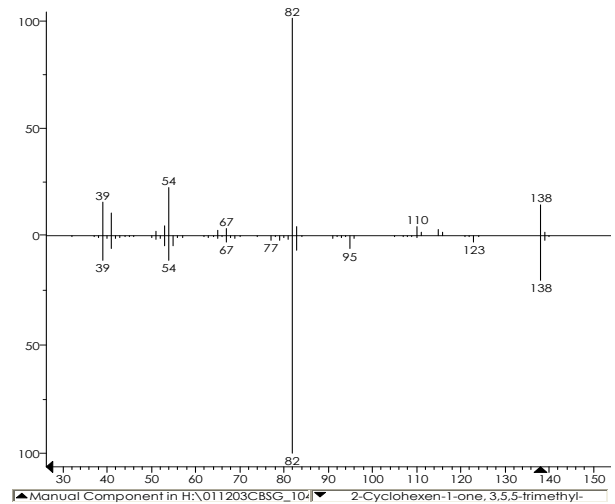
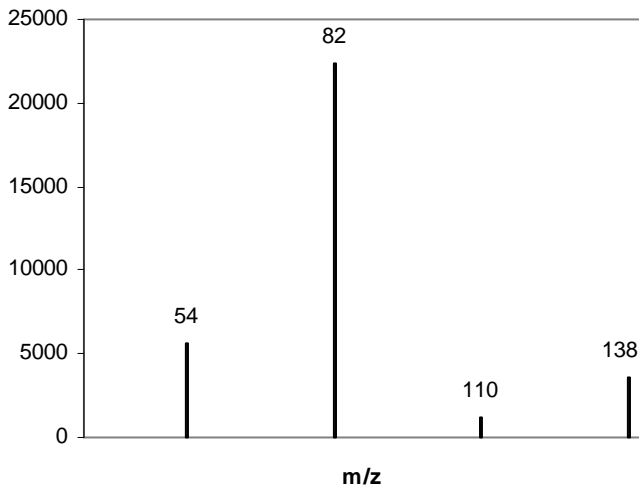


2-Caren-10-al (f.c. #280)

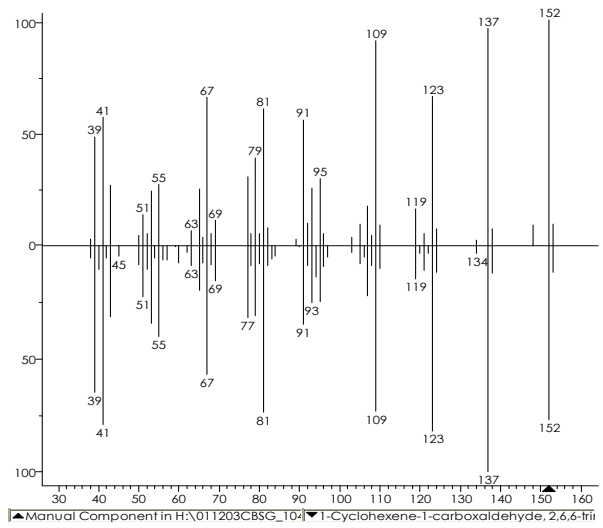
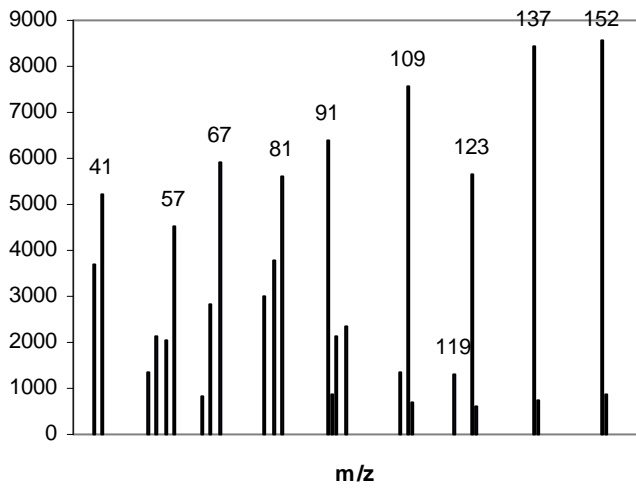


Cyclic carotenoid derivatives

α -Isophoron (f.c. #185)

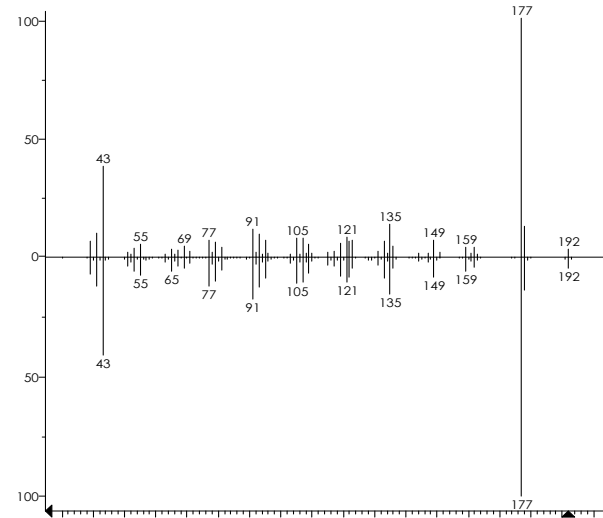
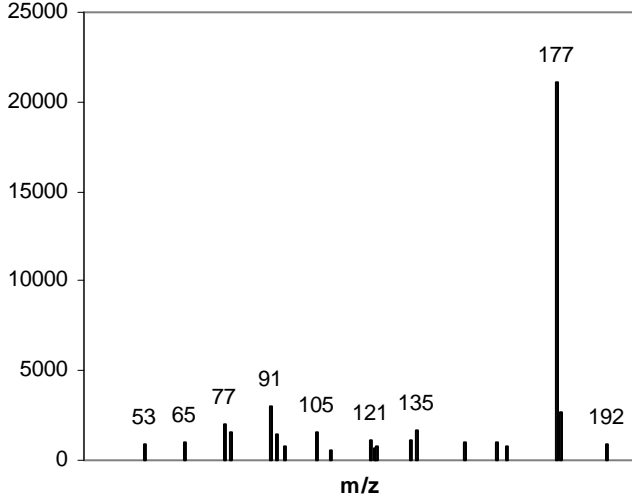


β -Cyclocitral (f.c. #243)



Manual Component in H:\011203CBSEG_104\1-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl

β -Ionone (f.c. #319)



Manual Component in F:\CBSEG3_VOLATILE\3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexyl)

β -Damascenone (f.c. #316)

