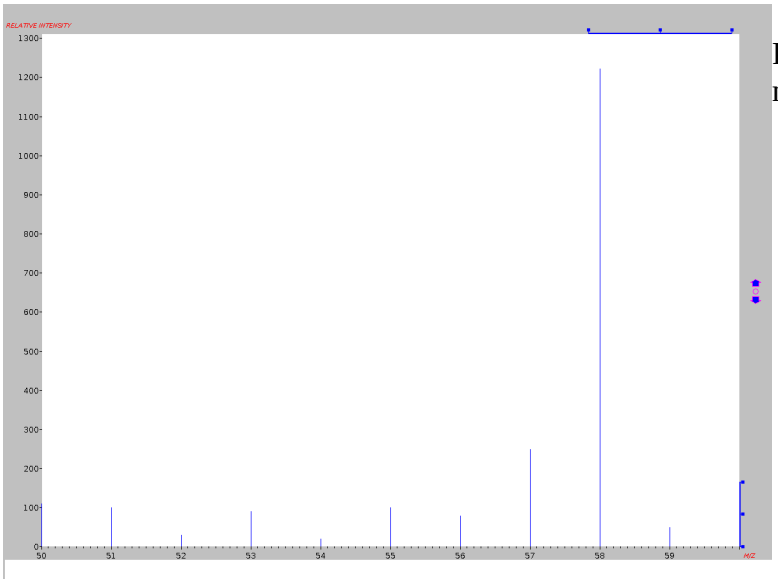
We will look at extracting different kinds of information from these spectra.

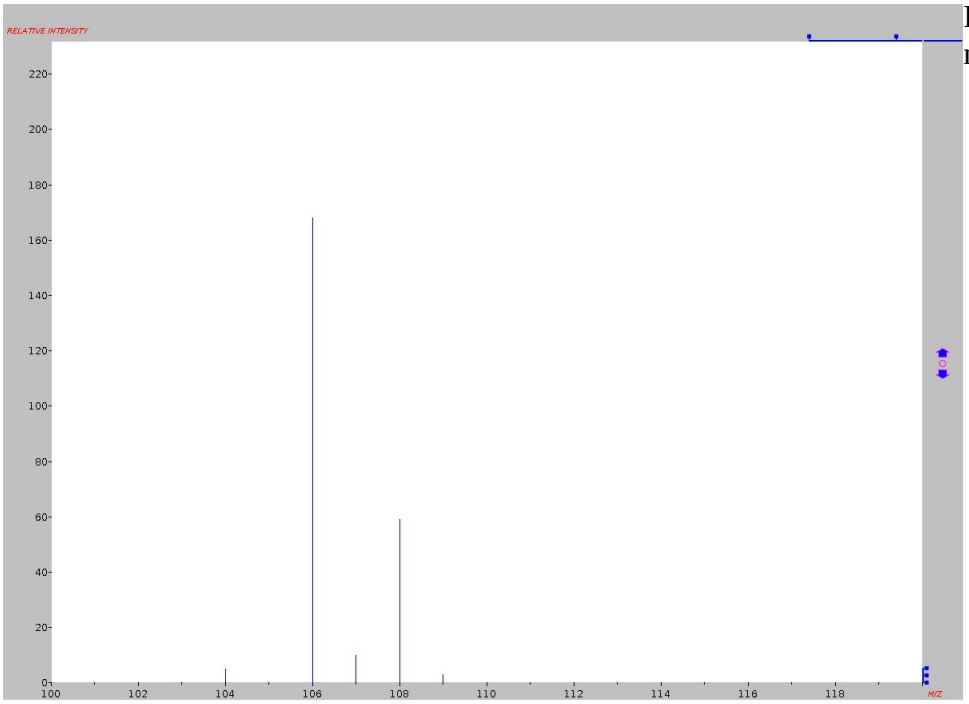
1. Find the molecular formula. First, estimate the number of carbons from the intensity of the $(M+1)^+$ peak. Subtract the mass of that many carbons from the M^+ peak mass. Then figure out the possible number of H's and O's.



Parent ion peaks:

m/z =	58	100
	59	4.1

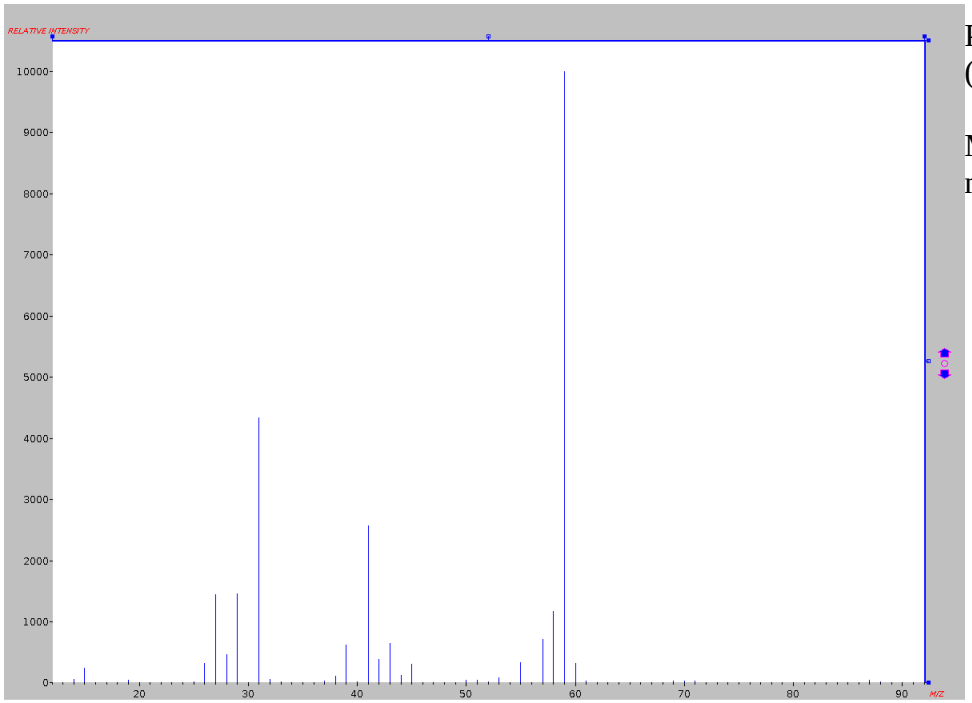
2. Molecular formula: atoms with multiple isotopes. First, identify the "unusual" element. Subtract its mass from the M+ peak mass. Then employ the same procedure as in #1 to find the number of C's, and the possible numbers of H's or O's.



Parent ion peaks:

m/z =		
	106	100
	107	5.95
	108	35.1
	109	1.78

3. Fragmentations.



Parent ion: m/z = 88.
$(M+1)^+$ too weak to see.

Major fragments:

m/z =		
59	100	
60	3.21	
41		
31		

A. Figure out the composition of the fragment at m/z = 59.

#C's = _____

Possible #H's = _____ _____ Are both reasonable?

Number of O's = _____

B. Figure out what neutral radical got lost: 88 – 59 = _____

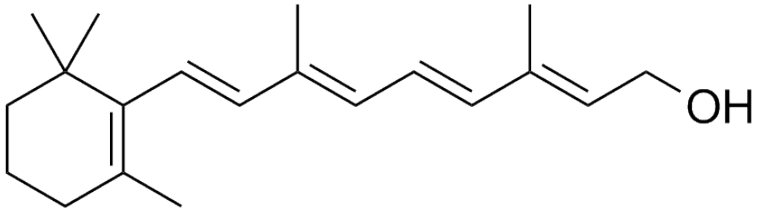
Possible formula = _____

C. Total molecular formula for m/z = 88: _____

Show some possible structures for this molecular formula that have the neutral radical fragment that got lost.

4. Vitamin A has a molar absorptivity in ethanol of 45,700 $M^{-1}cm^{-1}$ at λ_{max} = 326 nm.

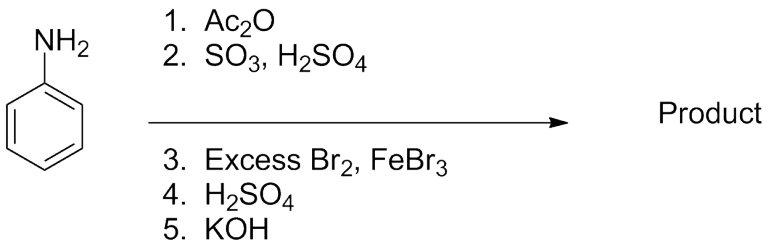
a. Circle the chromophore in the structure of Vitamin A below:



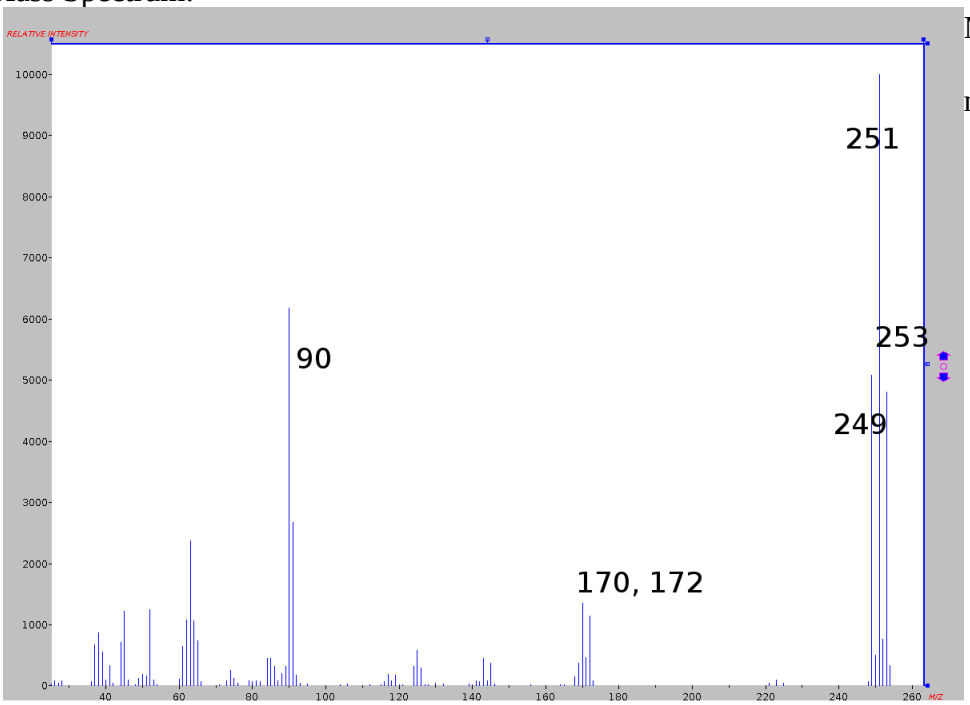
Vitamin A

b. Using Beer's Law (A = εbc), calculate the absorbance you should see if 286 μg are dissolved in 1 L ethanol. (Hint: the molecular weight of $C_{20}H_{30}O$ is 286 g/mol.)

5. The following multistep reaction sequence was performed. Spectra for the product are given; identify it and assign as many of the peaks in each spectrum as possible.



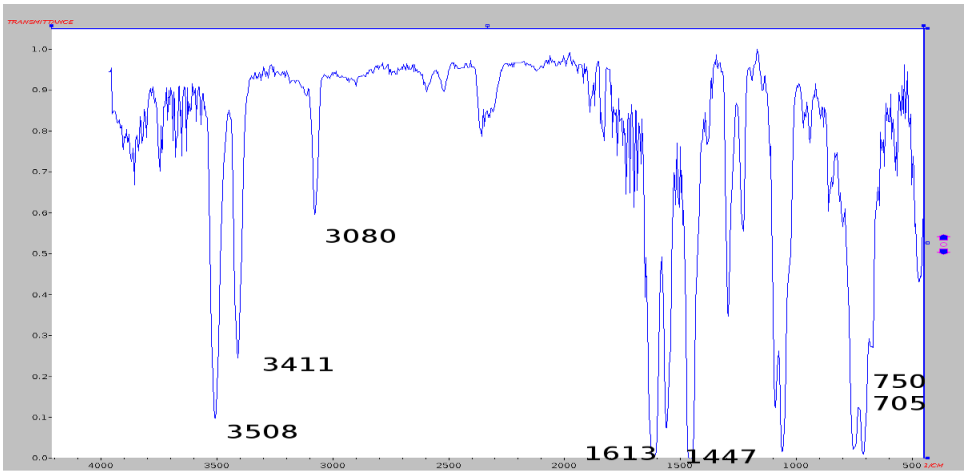
Mass Spectrum:



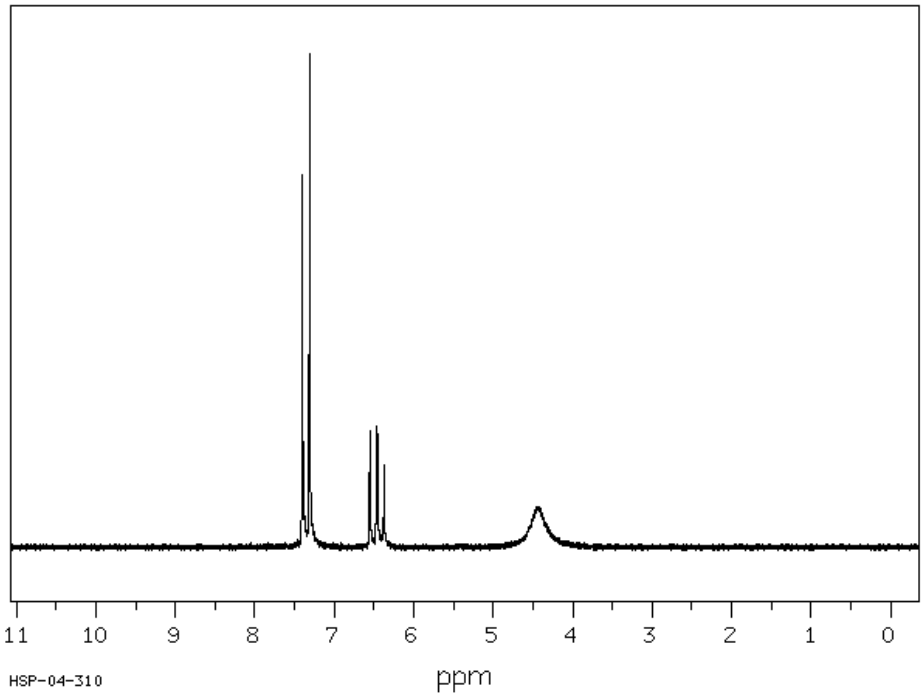
Major peaks:

m/z = 249 100
250 9.8
251 199
252 14.9
253 96
254 6.67

IR:

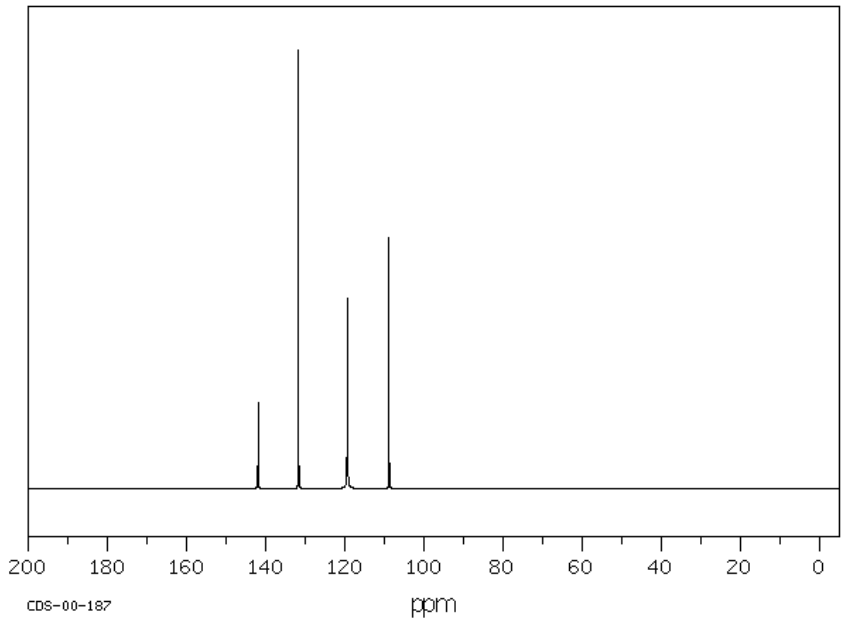


^{1}H NMR:



Integrals:
7.35: 2
6.47: 1
4.4: 2

^{13}C NMR:



141.93
131.71
119.33
108.83