S343 Quiz 1
9/11/14

Name_____

AI (or Lab Section) _____

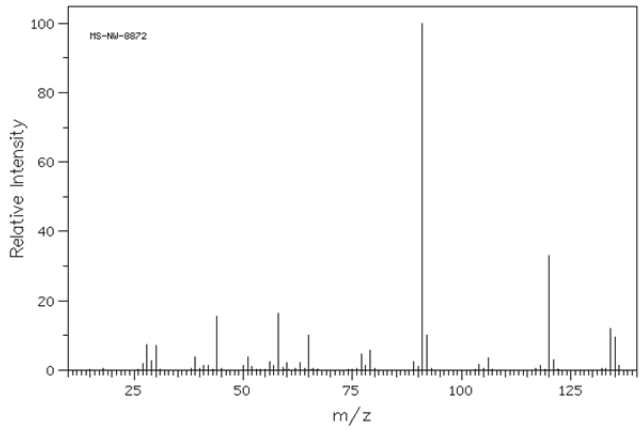
1. Answer the following questions about a molecule whose mass spectrometry data is given below (M = 135). (Hint: The rule of 13 is useful here.)

   a. Propose a molecular formula. _____

   b. What is the unsaturation number? _____

   c. What does the base peak suggest about the structure?

   d. Propose a ***reasonable*** structure for this compound. (Hint: after the base peak, m/z 120 is biggest)

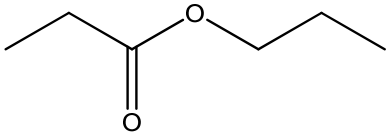


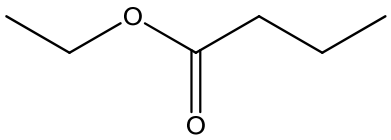
m/z	relative abundance	m/z	relative abundance	m/z	relative abundance	m/z	relative abundance
27.0	**1.9**	52.0	1.1	89.0	2.3	135.0 (M+)	9.5
28.0	**7.4**	56.0	2.3	90.0	1.1	136.0	1.0
29.0	**2.6**	57.0	1.4	91.0	100.0		
30.0	**7.2**	58.0	16.4	92.0	10.0		
39.0	**3.8**	60.0	2.2	104.0	1.6		
41.0	**1.4**	63.0	2.2	106.0	3.6		
42.0	**1.4**	65.0	10.0	118.0	1.4		
44.0	**15.5**	77.0	4.7	120.0	33.1		
50.0	**1.2**	78.0	1.4	121.0	3.1		
51.0	**3.8**	79.0	5.8	134.0	12.1		

2A. Propose the structure of an **alcohol** (M = 102) with major fragment ions at m/z 85, 73, 59. Support your answer with clearly drawn mechanisms that lead to these fragment ions.

B. In the MS of this alcohol, the molecular ion peak is very hard to distinguish. What would you do to obtain a spectrum in which it was more observable?

2. Explain how you would use mass spectrometry to distinguish between the following two isomers (M = 116). Be specific, and draw any important fragment ions that support your answer. (You do not need to draw fragmentation mechanisms.)





Supplemental data

The Natural Abundance of Isotopes Commonly Found in Organic Compounds

Element	Natural Abundance			
Carbon	^{12}C: 98.89%	^{13}C: 1.11%		
Hydrogen	^{1}H: 99.99%	^{2}H: 0.01%		
Nitrogen	^{14}N: 99.64%	^{15}N: 0.36%		
Oxygen	^{16}O: 99.76%	^{17}O: 0.04%	^{18}O: 0.20%	
Sulfur	^{32}S: 95.0%	^{33}S: 0.76%	^{34}S: 4.22%	^{36}S: 0.02%
Fluorine	^{19}F: 100%			
Chlorine	^{35}Cl: 75.77%		^{37}Cl: 24.23%	
Bromine	^{79}Br: 50.69%		^{81}Br: 49.31%	
Iodine	^{127}I: 100%			