

Assignment # 17

Organic 211

Fall 2020

Name: _____

1) Which molecular formula corresponds to a compound with a molecular ion (M^+) of 117 m/z in its mass spectrum? Explain your answer.

a) C_8H_7N

b) $C_7H_5N_2$

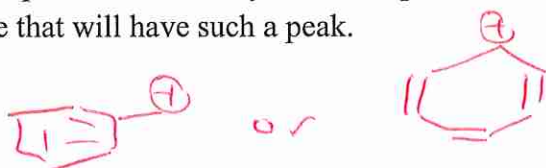
c) $C_7H_{14}F$

d) $C_6H_{13}O_2$

odd m^+
so odd #
of
nitrogens

2) You have a peak at m/z 91 in your mass spectrum. What does this represent? Give an example of a molecule that will have such a peak.

ion



C_7H_7

$$7 \times 12 = 84 + 7 = 91$$

3) You have a molecule that weighs 413. Give a possible molecular formula using the rule of 13. SHOW YOUR WORK.

means odd # of nitrogen, 3 for example

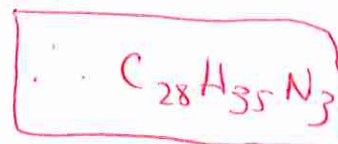
$$\frac{413}{13} = 31.769$$

$$\begin{array}{r} 413 \\ - 42 \\ \hline 371 \end{array}$$

$$\frac{371}{13} = 28.5384$$

$$\begin{array}{r} 28 \\ \times 12 \\ \hline 336 \end{array}$$

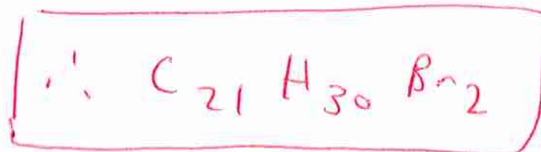
$$\begin{array}{r} 26 \\ 371 \\ - 336 \\ \hline 35 \end{array}$$



4) You have a molecule that weighs 440. It contains TWO bromines. Give a possible molecular formula using the rule of 13. SHOW YOUR WORK.

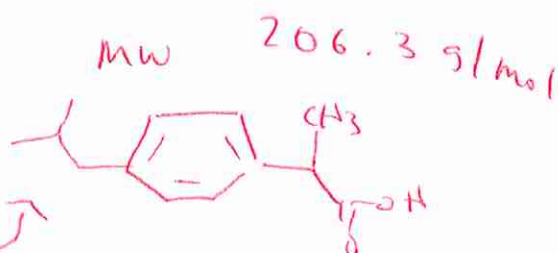
$$\begin{array}{r} R_r \\ (2 \times 79) \\ - 158 \\ \hline 282 \end{array} \quad \frac{282}{13} = 21.692$$

$$\begin{array}{r} 282 \\ - 252 \\ \hline 30H \end{array}$$



5) Given below is a great website for finding spectra.

http://riodb01.ibase.aist.go.jp/sdbs/cgi-bin/cre_index.cgi?lang=eng



a) Look up the mass spectrum of ibuprofen. (Need one now?)

b) What is the m/z of the base peak?

$$\boxed{163 - 100\%} \quad 206 - m+ - 45.9\%$$
$$161 - 96.9\%$$

c) Give the structure of the ion causing the base peak.

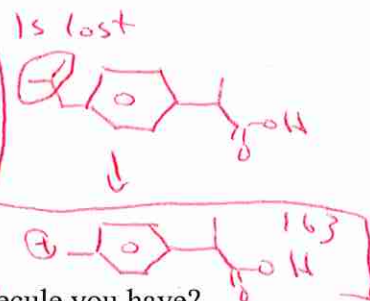
$$\begin{array}{r} 206 (m+) \\ - 163 (\text{base peak}) \\ \hline 43 \text{ lost} \end{array} \quad \rightarrow \quad \frac{43}{13} = 3.307$$

C_3H_7

$\begin{array}{r} 12 \\ \times 3 \\ \hline 36 \end{array} \quad \begin{array}{r} 43 \\ - 36 \\ \hline 7H \end{array}$

6) Your molecule has bromine in it. How could the mass spectrum prove this?

look at m+ peak. look at m+2 peak.
if they are equal, bromine present



7) N_2O and CO_2 have the same molecular weight. How could you tell which molecule you have?

- a) high resolution mass spectrum will identify which one it is by molecular weight since high resolution is 4 digits to right of decimal.
- b) inhale. if you laugh (N_2O - laughing gas) it is N_2O .