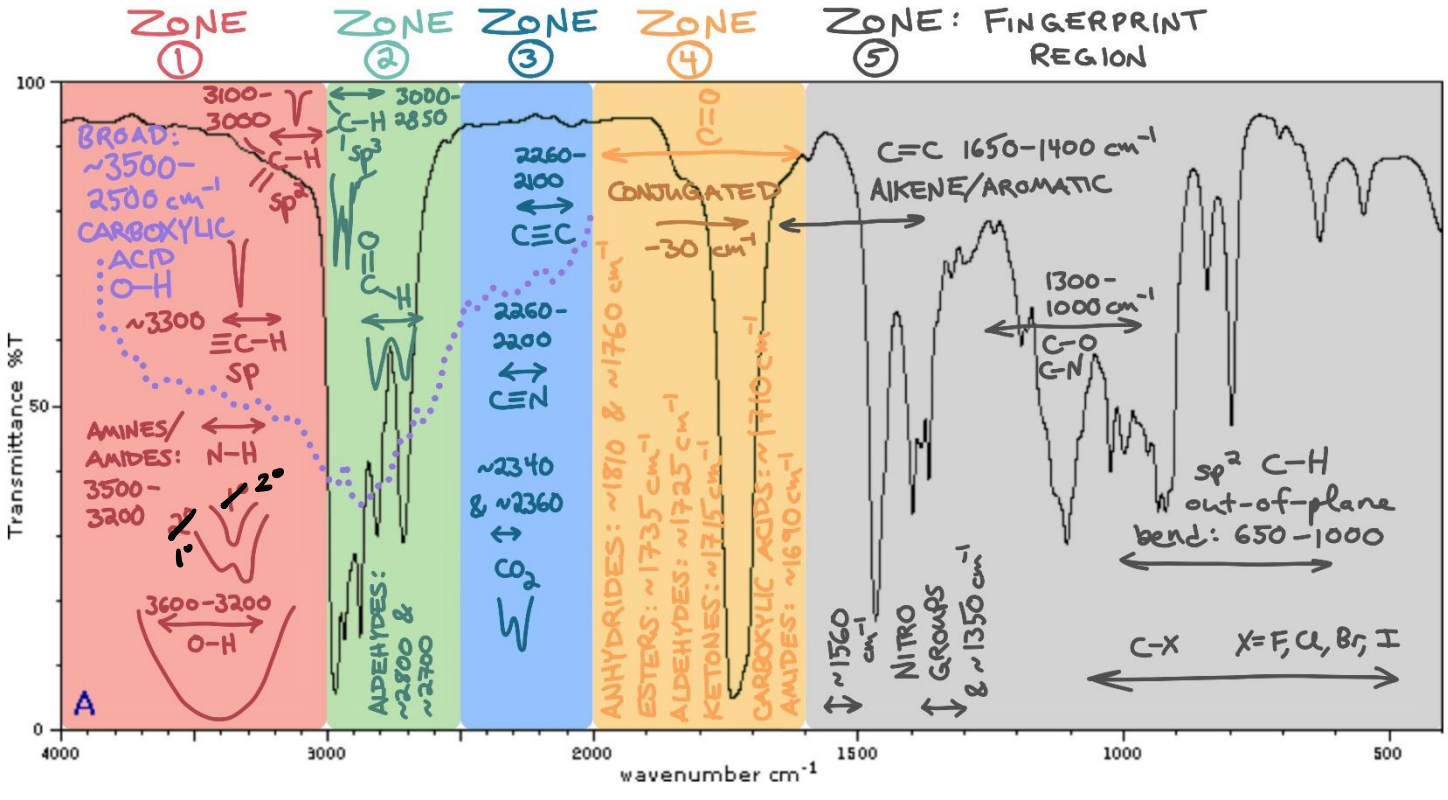
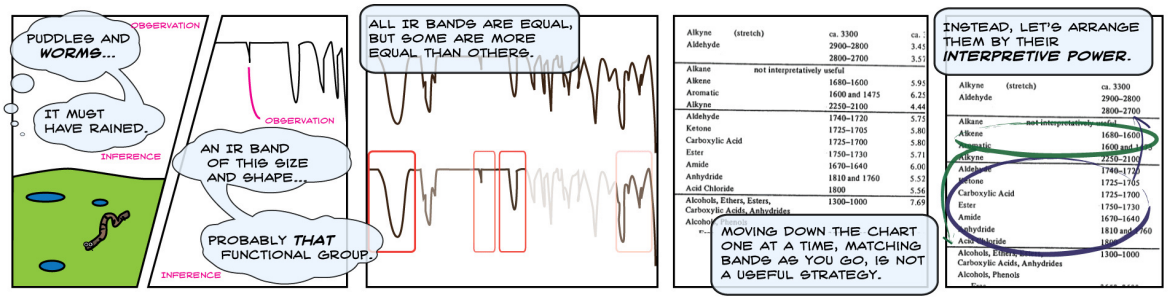
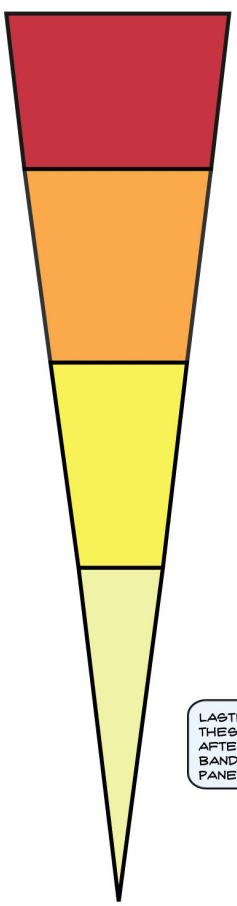
IDENTIFYING the MAJOR FUNCTIONAL GROUP:

1. Is a carbonyl present? **Check ZONE 4.** If no carbonyl is present, go to step 3.
   - **The C=O double bond gives rise to a strong absorption in ZONE 4: 2000-1600 cm^{-1}. This peak is often the strongest in the spectrum, and characteristic of the type of carbonyl present (see spectrum below).**
2. If C=O is present, check for additional peaks to confirm the following types of carbonyls:
   - **Anhydrides have two C=O absorptions near 1810 & 1760 cm^{-1}**
   - **Esters should also have C-O stretches in ZONE 5 around 1300-1100 cm^{-1} with medium intensity**
   - **Aldehydes should also have two signals in ZONE 2: ~2800 & ~2700 cm^{-1}**
   - **Carboxylic acids should have a broad signal that extends from ZONE 1 through ZONE 2: 3500-2500 cm^{-1}**
   - **Amides (primary & secondary) should have a signal in ZONE 1: 3500-3200 cm^{-1}**
3. If C=O is absent, check for:
   - **Alcohols/Phenols have a broad signal in ZONE 1: 3600-3200 cm^{-1}**
   - **Signals for amines also show up in ZONE 1: 3500-3200 cm^{-1}**
     i. **Primary amines (RNH_2) display 2 signals**
     ii. **Secondary amines (R_2NH) display 1 signal**
   - **Ethers have signals in ZONE 5 due to C-O stretch: 1300-1000 cm^{-1}**
4. Double bonds and/or aromatic rings:
   - **Phenyl and vinyl sp2 C-H stretches occur in ZONE 1 to the left of 3000 cm^{-1}**
   - **Alkenes display weak C=C stretching signals near 1650 cm^{-1}**
   - **Medium to strong signals from 1650-1400 cm^{-1} imply an aromatic ring**
5. sp Hybridized Triple bonds:
   - **Nitrile C≡N bonds display in ZONE 3 around 2250 cm^{-1}**
   - **Alkyne C≡C bonds display in ZONE 3 around 2150 cm^{-1}**
     i. **Terminal alkynes also have a sharp signal in ZONE 1 around 3300 cm^{-1}**
6. Nitro groups, NO_2:
   - **N=O stretches observed as two signals in ZONE 5 around 1560 & 1350 cm-1**
7. Alkanes:
   - **Main signals for sp3 hybridized C-H bonds are in ZONE 2 just below 3000 cm^{-1}**

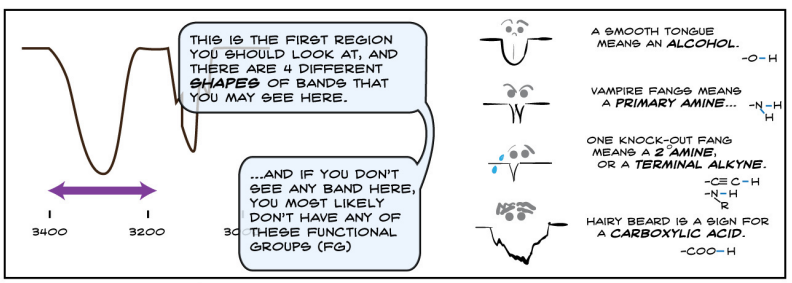


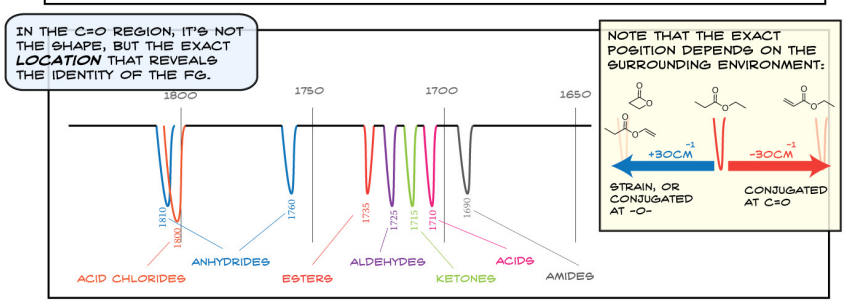


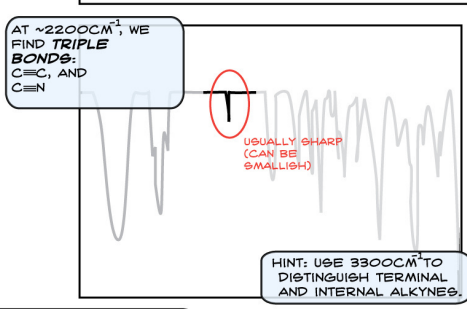
GREAT INTERPRETIVE POWER



WIMPY INTERPRETIVE POWER







Interpreting IR spectra

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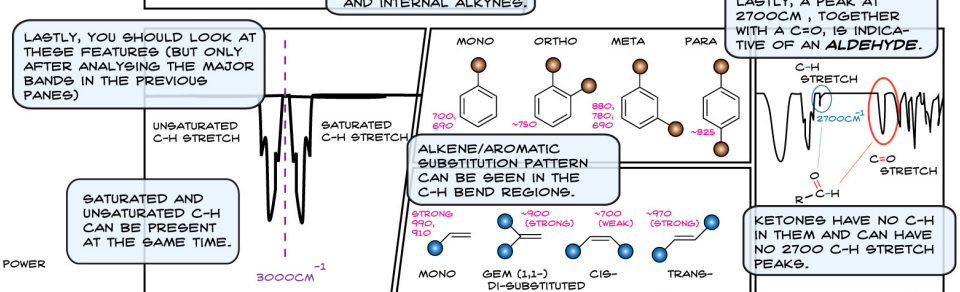


WE LOOKED AT THESE LAST BECAUSE THEY CAN BE AMBIGUOUS TO INTERPRET, OR THEY HAVE ONLY A NARROW NICHE OF USEFULNESS.

NOTES

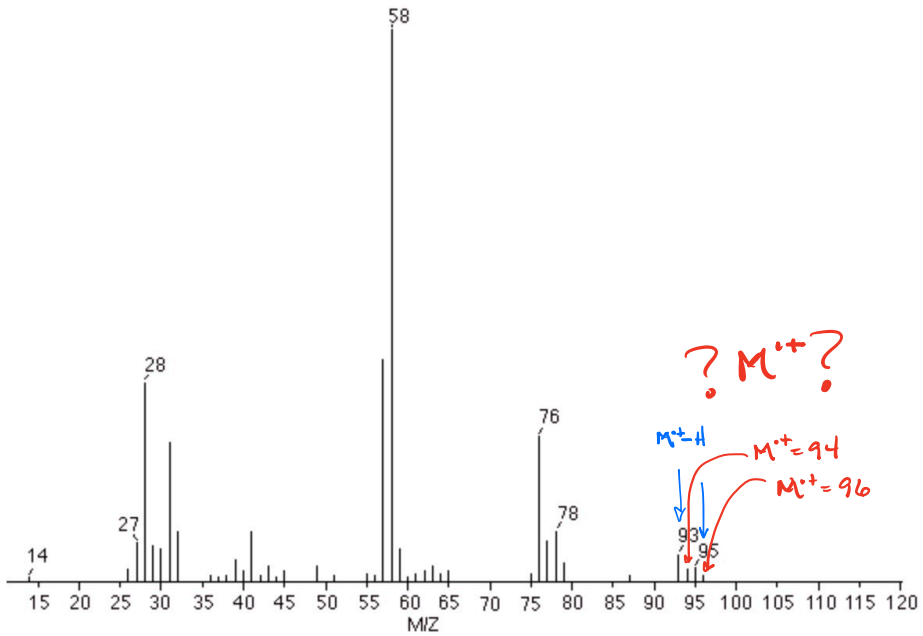
** IF YOU'RE NOT SURE WHAT THE DIFFERENCE BETWEEN AN ACID AND AN ALCOHOL IS, DO THE QUICK "FUNCTIONAL GROUP IDENTIFICATION" EXERCISE.

** ...IF YOU HAVE ONE FG. TWO 2° AMINE WOULD LOOK LIKE A 1 AMINE.

CoOP #3, Problem 3

Mass Spec

Problem 3: Positive EI Mass Spectrum



IR - shows strong Alcohol @ 3300 cm⁻¹

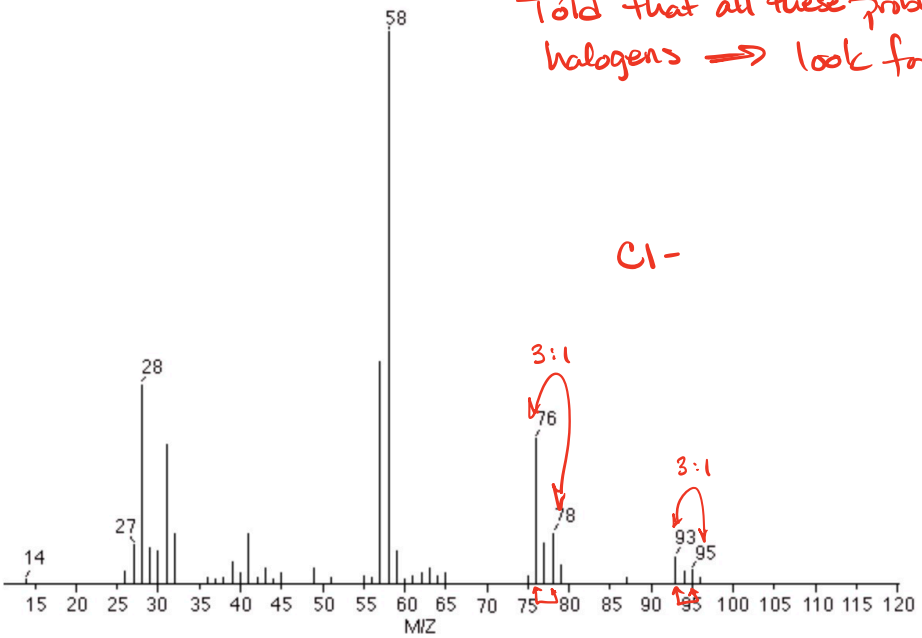
Mass Spec R-OH

Very unstable M·+ often small or missing

M/z

Loss of 1

Problem 3: Positive EI Mass Spectrum



Told that all these problems have halogens ⇒ look for

1:1 3:1

Br Cl

2amu 2amu

Cl-

HNMR H_7

CNMR C_3

min #

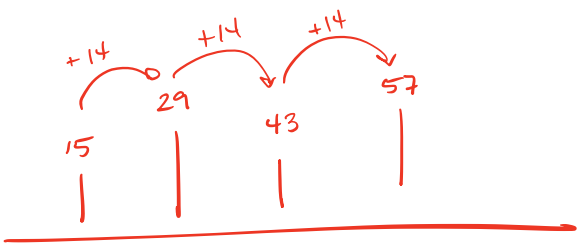
Could be more

$C_3H_7{}^{35}ClO = 94$ ✓ 3

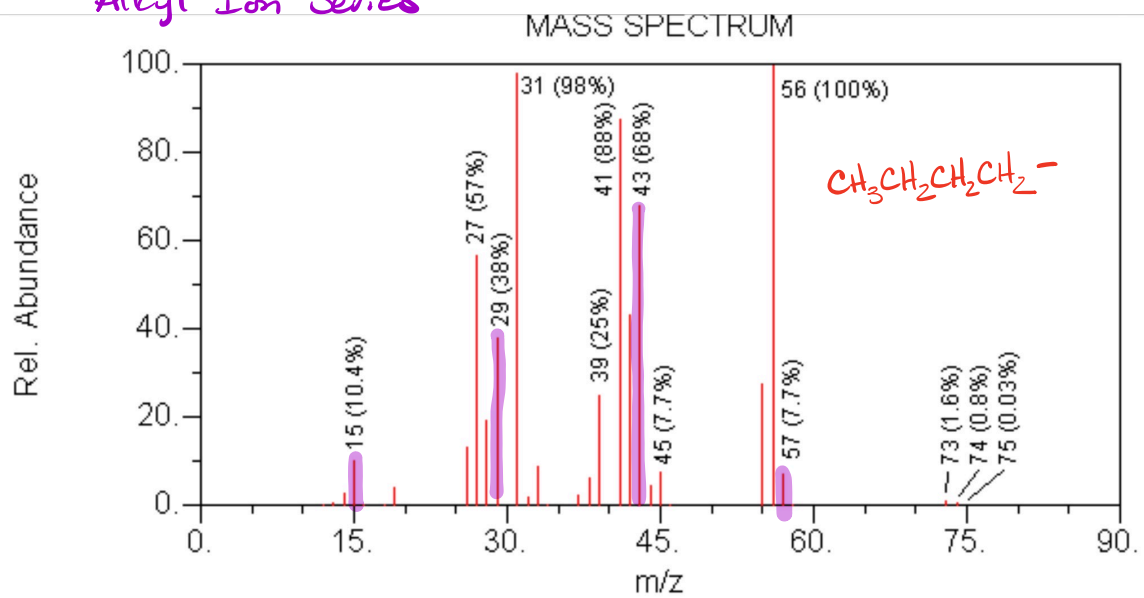
$C_3H_7{}^{37}ClO = 96$ ✓ 1

Ratio

Mass Spec Alkyl ion Series



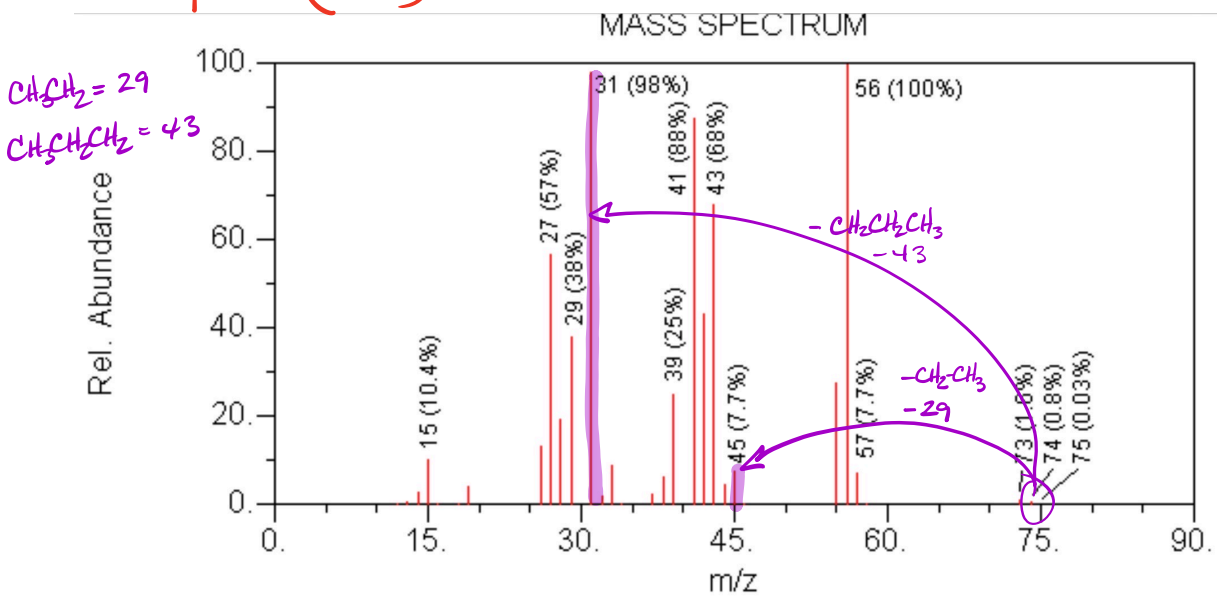
Alkyl Ion Series



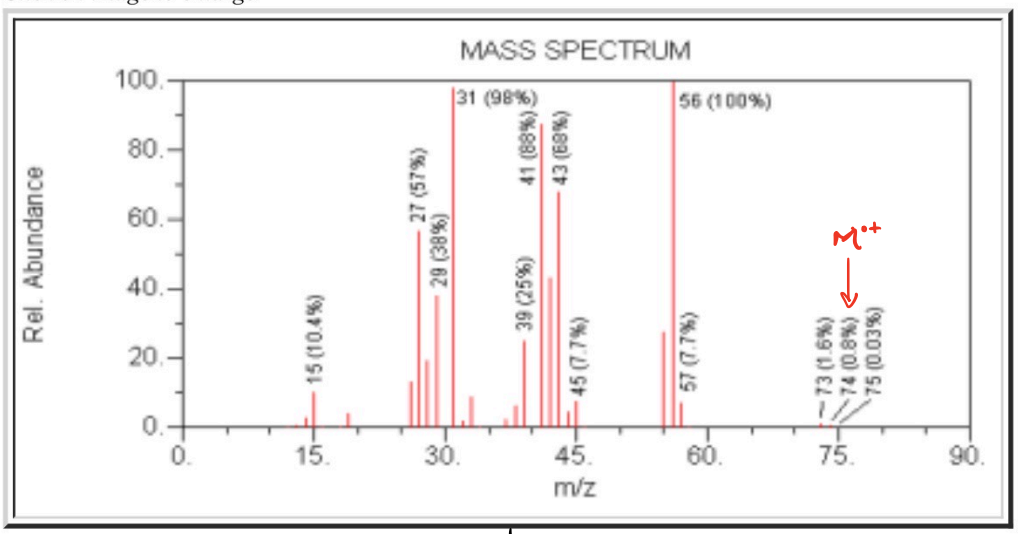
Alkyl Ion(Loss) Series

$CH_3CH_2 = 29$

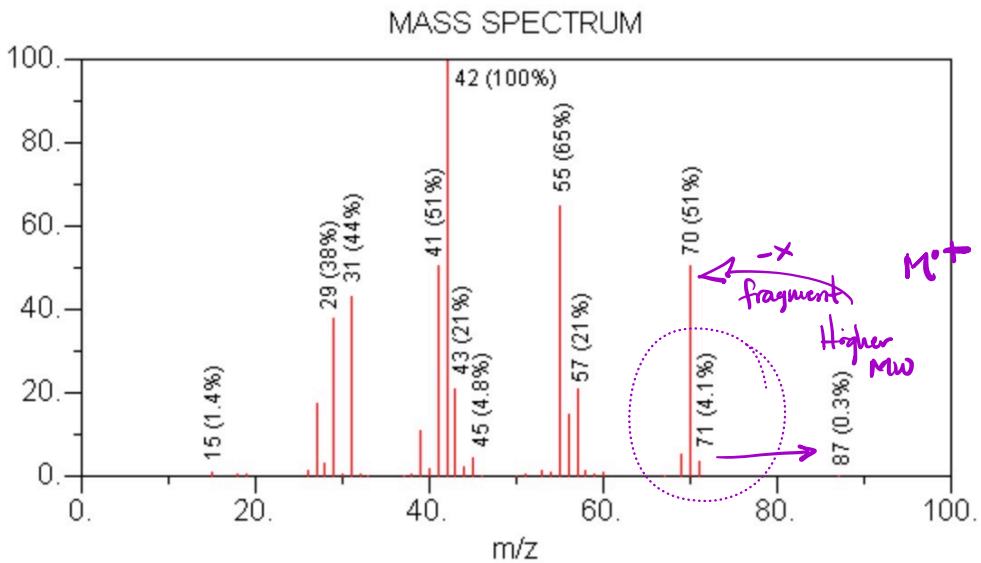
$CH_3CH_2CH_2 = 43$



Click on image to enlarge



- ○ **a)** 2-methyl-2-propanol — $C_4H_{10}O$ 74 — No straight chain
- ⊗ **b)** 1-butanol — $C_4H_{10}O$ 74 — straight chain
- ○ **c)** 2-butanol — $C_4H_{10}O$ 74
- ○ **d)** 1-pentanol — ~~$C_5H_{12}O$ 88~~
- ○ **e)** 2-methyl-1-propanol — $C_4H_{10}O$ 74 — No straight chain



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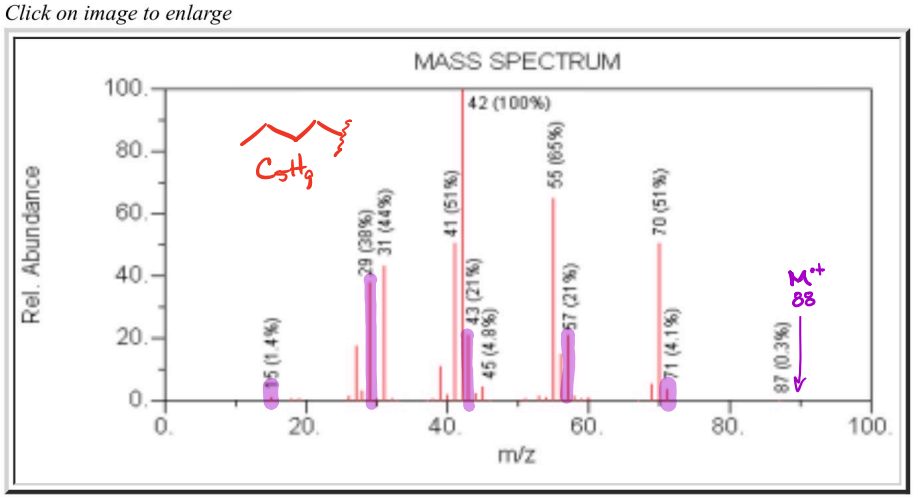
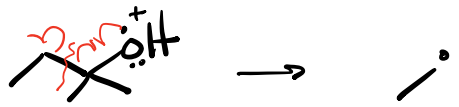


- ○ **a)** 1-hexanol — $C_6H_{14}O$ — 102
- ⊗ **b)** 1-pentanol — $C_5H_{12}O$ — 88
- ○ **c)** 2-methyl-2-butanol — $C_5H_{12}O$ — 88
- ○ **d)** 2-pentanol — $C_5H_{12}O$ — 88
- ○ **e)** 1-butanol — $C_4H_{10}O$ — 74



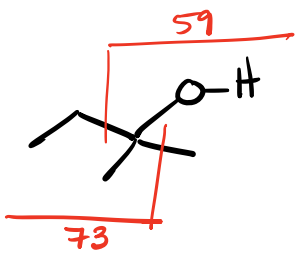
M/z = 59

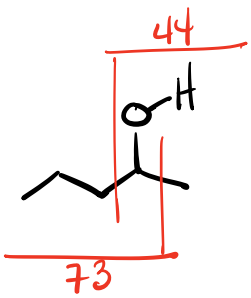
C_3H_7O

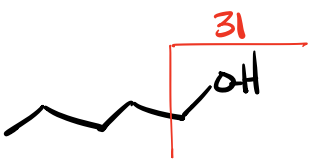
$\dot{C}H_3$

C_4H_9O

M/z = 73







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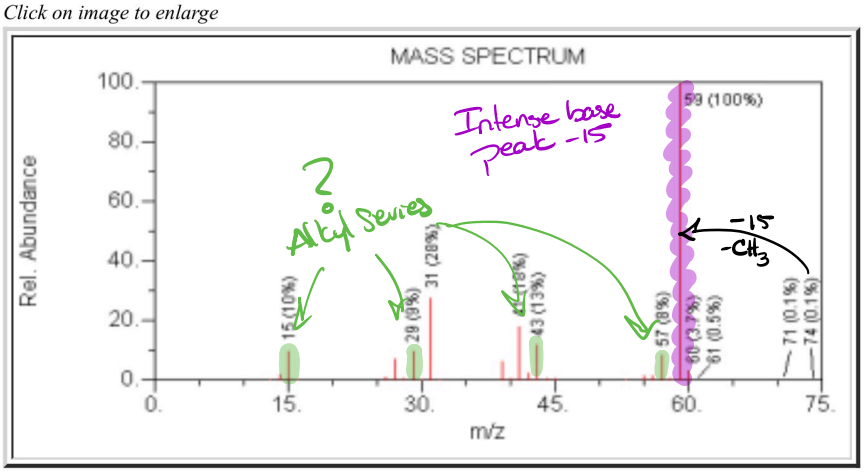

- a) 2-methyl-2-butanol
- b) 2-methyl-2-propanol
- c) 2-butanol
- d) 1-butanol
- e) 2-methyl-1-propanol