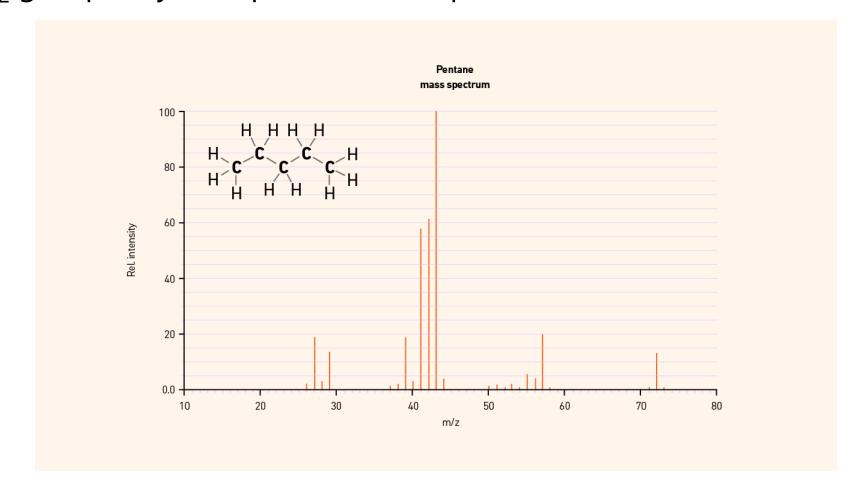# *Biomolecules*
Answer In-class activity 5: MS Spectroscopy

ELEC-E3260

In-Class Activity

Here you have the mass spectrum of the pentane (C_5H_{12}), consisting of CH_3 and CH_2 groups, try to explain me the spectrum obtained.

- Pentane has the chemical formula C_5H_{12}. The approximate mass of the molecule is therefore ((12 x 5) + (1 x 12)), or **72 amu**.

- Notice that on the mass spectrum a peak with relative intensity of ~ 10% is observed at m/z = 72 amu. **This is the molecular peak**. The entire molecule has been ionized in the source as a single entity without any fragmentation.

But what of the other, stronger peaks?

- These are the result of fragmentation during the ionization process of pentane.
- How can the next heaviest mass observed be interpreted (at m/z = 57 amu with ~ 20% relative intensity)?
- With a bit of math, we can propose it might be C_4H_9, which would suggest one of the CH_3 groups was fragmented off during the ionization process, leaving the C_4H_9 fragment molecular ion.
- Similarly, the strongest signal observed at m/z = 43 amu can be interpreted as C_3H_7, meaning a C_2H_5 molecule was fragmented. This is the equivalent of one of the CH_3 and CH_2 groups.
- Note that there are also strong lines at m/z = 41 and 42. These are due to extra Hs being stripped from the C_3H_7 molecular ion during fragmentation.