Here are a list of steps to follow when interpreting a mass spectrum. This simplified list will help you to interpret many spectra, however there are other mechanisms of fragmentation which cannot be covered in this brief tutorial.

Steps to interpret a mass spectrum

1. Look for the molecular ion peak.
   - This peak (if it appears) will be the highest mass peak in the spectrum, except for isotope peaks.
   - Nominal MW (meaning=rounded off) will be an even number for compounds containing only C, H, O, S, Si.
   - Nominal MW will be an odd number if the compound also contains an odd number of N (1, 3, ...).

2. Try to calculate the molecular formula:
   - The isotope peaks can be very useful, and are best explained with an example.
     - Carbon 12 has an isotope, carbon 13. Their abundances are $^{12}\text{C}=100\%$, $^{13}\text{C}=1.1\%$. This means that for every 100 ($^{12}\text{C}$) atoms there are 1.1 ($^{13}\text{C}$) atoms.
     - If a compound contains 6 carbons, then each atom has a 1.1% abundance of $^{13}\text{C}$.
     - Therefore, if the molecular ion peak is 100%, then the isotope peak (1 mass unit higher) would be $6 \times 1.1\% = 6.6\%$.
     - If the molecular ion peak is not 100% then you can calculate the relative abundance of the isotope peak to the ion peak. For example, if the molecular ion peak were 34% and the isotope peak 2.3%: \( \frac{2.3}{34} \times 100 = 6.8\% \). 6.8% is the relative abundance of the isotope peak to the ion peak. Next, divide the relative abundance by the isotope abundance: $\frac{6.8}{1.1}=6$ carbons.
   - Follow this order when looking for information provided by isotopes: (A simplified table of isotopes is provided in the introduction, more detailed tables can be found in chemistry texts.)
     - Look for A+2 elements: O, Si, S, Cl, Br
     - Look for A+1 elements: C, N
     - "A" elements: H, F, P, I

3. Calculate the total number of rings plus double bonds:
   - For the molecular formula: C<sub>x</sub>H<sub>y</sub>N<sub>z</sub>O<sub>n</sub>
     - rings + double bonds = \( x - \frac{1}{2}y + \frac{1}{2}z + 1 \)

4. Postulate the molecular structure consistent with abundance and m/z of fragments.
   - More information on specific fragmentation can be found in the quiz for each functional group.

Contributors