Figure 1 and the isotope abundance data from Table 1, we can see that there are 1.08 $^{13}\text{C}$ atoms for every 100 $^{12}\text{C}$ atoms, and the $^{13}\text{C}$ peak will be 1.08% as large as the $^{12}\text{C}$ peak.

The example above is simple, but the same methods can be applied to determine isotope peaks in more complicated molecules as well. The molecule $\text{C}_4\text{Br}_1\text{O}_2\text{H}_5$ has several isotope effects: $^{13}\text{C}$, $^2\text{H}$, $^{81}\text{Br}$, $^{17}\text{O}$, and $^{18}\text{O}$ all must be taken into account. First we will look at the $(\text{M}+1)^+$ peak in comparison with the $\text{M}^+$ peak. Only isotopes that will increase the value of $\text{M}$ by 1 must be taken into consideration here – since $^{81}\text{Br}$ and $^{18}\text{O}$ would both increase $\text{M}$ by 2, they can be ignored (the most abundant isotopes for Br and O are $^{79}\text{Br}$ and $^{16}\text{O}$). Like the previous example, there are 1.08 $^{13}\text{C}$ atoms for every 100 $^{12}\text{C}$ atoms. However, there are 4 carbon atoms in our molecule, and any one of them being a $^{13}\text{C}$ atom would result in a molecule with mass $(\text{M}+1)$. So it is necessary to multiply the probability of an atom being a $^{13}\text{C}$ atom by the number of C atoms in the molecule. Therefore, we have:

$$4\text{C} \times 1.08 = 4.32 = \text{molecules with a } ^{13}\text{C} \text{ atom per 100 molecules}$$

We can repeat this analysis for $^2\text{H}$ and $^{17}\text{O}$:

$$5\text{H} \times 0.015 = 0.075 = \text{molecules with a } ^2\text{H} \text{ atom per 100 molecules}$$

$$2\text{O} \times 0.04 = 0.08 = \text{molecules with a } ^{17}\text{O} \text{ atom per 100 molecules}$$

Any of the three isotopes, $^{13}\text{C}$, $^2\text{H}$, or $^{17}\text{O}$ occurring in our molecule would result in an $(\text{M}+1)^+$ peak. To get the ratio of $(\text{M}+1)^+/\text{M}^+$, we need to add all three probabilities:

$$4.32 + 0.075 + 0.08 = 4.475 = (\text{M}+1)^+ \text{ molecules per 100 } \text{M}^+ \text{ molecules}$$

We can say then that the $(\text{M}+1)^+$ peak is 4.475% as high as the $\text{M}^+$ peak.

A similar analysis can be easily repeated for $(\text{M}+2)^+$:
$1\text{Br} \times 98 = 98 = \text{molecules with an } ^{81}\text{Br \ molecule per 100 molecules}$

$2\text{O} \times 0.2 = 0.4 = \text{molecules with an } ^{18}\text{O \ molecule per 100 molecules}$

$98 + 0.4 = 98.4 = (M+2)^+ \text{ molecules per 100 } M^+ \text{ molecules}$

The $(M + 2)^+$ peak is therefore 98.4% as tall as the $M^+$ peak.

This method is useful because using isotopic differences, it is possible to differentiate two molecules of identical mass numbers.

Contributors and Attributions

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