Mass Spectrometry walkthrough:

Starting with a graph find M, M+1, and M+2

From the graph above look for M first. It is the m/z that is furthest Intensities to the right. M stands for the mass of the molecule that is being tested. The intensities that are left of the M are fragmented parts of the molecule that have broken down and are unimportant to figuring out the chemical formula.

For the graph above, M is 98 because it is part of a set of intensities that is furthest to the right, but is also the higher point in the set. The Intensities to the right of M are isotopes of M that appear naturally (ex Br) in fixed percentages. For example, carbon 12 appears about 99% while carbon 13 appears about 1.1%

Now that M, M+1, and M+2 have been identified, make sure that they are rescaled so that M:100% in the example above: M:100::M+1:Rescaled M+1

Rescaled M+1/1.1% = # of Carbons

Rescaled M+2: if 4% then presence of sulfur  
if 33% then presence of chlorine  
if 100% then presence of bromine

How to determine if multiple Sulfur, Chlorine, or Bromine?  
If there are multiple atoms, then the chances for their isotopes are respectively the same. To make it easier, list out all the isotopes of these atoms

For example: CH₂Cl₂ Natural Abundances (Given in table)  
M: CH₂³⁵Cl₂:75% x 75% = .5625  
M+2: CH₂³⁵Cl³⁷Cl:75% x 25% = .1875  
M+2: CH₂³⁷Cl³⁵Cl:25% x 75% = .1875  
Total M+2:.1875+.1875=.375  
M+4: CH₂³⁷Cl₂:25% x 25% = .0625
Now, rescale these values of M to 100% and rest accordingly.

\[ M(56.25\%):100::M+2(37.5\%):\text{Rescaled M+2 (?)} \]

Rescaled M+2: 66.67%

Now we can conclude that the M+2 Intensity will be 2/3’s the height of the M bar if there are two Chlorines. This methodology can be applied to Sulfur and Bromine to find their respective heights of M+2 in relation to M when there are more than one of these atoms. (the M+1 bar will still only include information about carbon)

In the reverse, if we are given the mass spectrometry data and M:100%; and M+2:66.67%, then there is a possibility that there are two Chlorines. However, there could be other combinations of Sulfur, Chloride, and Bromine to make up the 66.67%.

Finally, general information that is in Lecture supplement.
Mass Spectrometry gives data about:

- M : Molecular weight
- M+1: Number of carbon
- M+2: presence of Sulfur, Chlorine, or Bromide

Atoms that are not covered by Mass Spectrometry: Oxygen, Nitrogen*, and Hydrogen**

Use elimination and Brute Force algorithm skills to create a reasonable formula that fits into above criteria.

*Nitrogen Rule: If the (M) molecular weight is odd, then number of Nitrogen is odd; if molecular weight is even, then the number of Nitrogen is even

**Hydrogen Rule: Pi bond reduces max hydrogen count by two. Each ring decreases max hydrogen count by two. Max number of H: 2(#of Carbon) - 1 DBE per pi bond or ring (double bond 1DBE; triple bond 2DBE, benzene ring 4DBE)

Using all previously calculated and given data use this equation:

\[ \text{DBE} = \#\text{of Carbon} - (\#\text{of Hydrogen}/2) + (\#\text{of Nitrogen}/2) + (#\text{of Nitrogen}) + 1 \]

DBE can be used to predict possible structures and functional groups.

picture from http://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/Spectrpy/MassSpec/masspec1.htm
all other information synthesized from lecture and 14c Lecture Supplement