

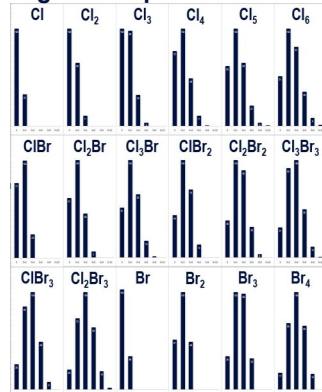
GC/MS (EI) Interpretation Quick Reference Guide

With the advent of modern GC/MS instruments and software when analysing unknowns, there is a lack of skills and understanding of how compounds fragment. Also required is a knowledge of how GC/MS libraries are compiled and the options for the search algorithms. If this is not fully understood the result could be an unmatched spectra or of more concern, false identification of unknown compounds.

Library Considerations

- 1st library match may not be correct.
- The compound may not be in the library(s) being searched.
- The acquisition mass range may not match library mass range.
- Different library search algorithms may provide different compound matches.
- Smaller peaks may require background subtraction before library search.
- Create your own libraries from data acquired on your instrumentation.

Halogen Isotopic Abundances



EI Interpretation Strategy

- Note general appearance of spectrum to see if it is interpretable.
- Select a candidate peak for the molecular ion (M^+).
- Examine spectrum for peak clusters of characteristic isotopic patterns.
- Test M^+ candidate by searching for peaks corresponding to reasonable loss.
- Look for characteristic low-mass fragment ions.
- Compare spectrum to reference spectra:
 - using compilations in published references
 - using computerized search of reference spectra
- Spectral interpretation must be reconciled with:
 - retention times of nearby peaks in relation to compound indices
 - all other information about the sample.
- Check interpretation by obtaining a spectrum of pure compound under the same instrumental conditions.

Molecular Ion (M^+) Considerations

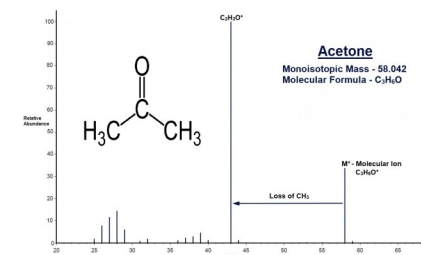
- If compound is known, molecular ion will have an m/z value equal to the sum of the atomic masses of the most abundant isotope of each element that comprises the molecule.
- The M^+ peak must be the highest m/z value peak of significance (non-background, non isotope).
- The nominal molecular weight or m/z value for the molecular ion will be an even number for any compound containing only C, H, O, S, Si, P and halogens.
- Fragment ions derived via homolytic fission from these ions will have an odd m/z value.
- Fragment ions derived from these molecular ions (even mass) via expulsion of neutral components (e.g., H_2O , CO , ethylene, etc.) will themselves have an even value of m/z .
- Nitrogen Rule: A compound containing an odd number of nitrogen atoms in addition to C, H, O, S, Si, P and halogens will have an odd molecular weight.
- No fragment ion may contain a larger number of atoms of any particular element than the M^+ .

Conclusion

If these guidelines are adhered to you are more likely to avoid misidentification of unknown compounds and produce more accurate data.

ChromSolutions Ltd

What we offer at ChromSolutions is our wealth of experience in analytical instrument sales and support (over 110 years distributed through the members of our company). We use this experience and extensive libraries to provide concise guidance to GC/MS interpretation. This can be done by providing remote learning, or access to your GC/MS data to ensure the best possible identification of unknown compounds.



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