CHAPTER OVERVIEW

6: INTERPRETATION

Although mass spectrometry is a very sensitive instrumental technique, there are other techniques with picogram detection limits. In addition to sensitivity, however, mass spectrometry also is also useful for identifying the chemical structure of this picogram sample. Since the mass spectrum is a fingerprint of the molecular structure, comparison to a computer databases can be used to identify an unknown compound. This is often done using Probability Based Matching (PBM), a popular pattern recognition technique. Although these computer searches are convenient and powerful, it is important to understand how to interpret a mass spectrum. A computer only compares the unknown spectrum to the library spectra and offers a selection of compounds in the database that produce similar spectra. This computer search is very useful and it makes interpretation much easier, but there are limits to the computer search.

Molecular structure is important for understanding mass spectral interpretation. To get the most from this section, draw out the structures of the molecules discussed. During the discussion find which bonds break and calculate the mass of the fragments. Actively reading this section will result in a much greater understanding of and appreciation for mass spectrometry. You can interpret the spectrum but it will take some effort. One common mistake made in mass spectrometry is to blindly trust the results of a computer library match. You need to learn how to interpret and understand the mass spectrum to effectively use these computer searches. This section should help you get started.