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Identification and Characterization of New Drugs Using Mass Spectrometry

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Mass spectrometer can be used in 3 principal ways: firstly, to measure the molecular weights with very high accuracy; from these can be deduced exact molecular formulae. Secondly, to detect within a molecule the places at which it prefers to fragment; from this can be deduced the presence of functional groups within the molecule. And thirdly, as a method for identifying drug molecules by comparison of their mass spectra with libraries of digitized mass spectra of known compounds. Molecular ion gives highly useful information about the identity of the drug molecule. Fragmentation pattern gives further information about the structure of the drug molecule. All fragment ions are, however, not of equal significance to assign the structure to a compound. Intensity of the molecular ion peak in a mass spectrum depends on the type of the compound. Mass spectra cannot be interpreted if they contain any misinformation. Unfortunately, even referred journals and carefully edited collections of the standard spectra sometimes contains spectra that fail to meet this criterion. Some compounds e.g., alcohols may fail to give a visible molecular ion peak. Judging whether or not a mass spectrum is credible is sometimes the most critical step in its interpretation. Most EI mass spectrometers in use today lack sufficient resolving power to provide accurate mass measurement for the determination of elemental composition. However, the elemental composition of an ion can sometimes be determined from the ratios of the peak intensities of the isotope peaks for that ion to the intensity of the nominal mass peak. Some typical features may be helpful i.e., if the M+2 peak of the parent ion looks larger than the M+1 peak, the compound might contain S,Cl or Br. When there is a larger gap and a peak at 127, iodine may be present. The intensity of the M+1 peak can be used to know the number of carbons well as nitrogen atoms. In the absence of nitrogen, the maximum number of carbaon atoms can be calculated by dividing the relative intensity of the M+1 peak by 1.1. Thus, e.g., a molecule with 12 carbon atoms will display a M+1 peak of 13.2 per cent. In case nitrogen is present its contribution to the M+1 peak will amount of 0.4 X number of nitrogen atoms. This quantity must be subtracted from the measured relative intensity of the M+1 peak to know the number of carbon atoms. When in a compound Cl, Br, S or Si is present loss of a proton from the M+2 is likely to enhance the intensity of the M+1 peak. The number of nitrogen atoms present can be deduced with the help of nitrogen rule. In this talk we will address, how to identify different drug molecules using mass spectrophomter with relevant examples.