A simple definition of a Mass Spectrometer

- A Mass Spectrometer is an analytical instrument that can separate charged molecules according to their mass to charge ratio.
- The mass spectrometer can answer the questions what is in the sample (qualitative structural information) and how much is present (quantitative determination) for a very wide range of samples at high sensitivity.

Components of a Mass Spectrometer

- 1- Vacuum System
- 2- Atmosphere

How are mass spectra produced ?

• Ions are produced in the source and are transferred into the mass analyser.

- They are separated according to their mass/charge ratio in the mass analyser (e.g. Quadrupole, Ion Trap)
- Ions of the various m/z values exit the analyser and are counted by the detector.

What is a Mass Spectrum ?

A mass spectrum is the relative abundance of ions

of different m/z produced in an ion source



- 1-a chemical fingerprint
- 2-Molecular weight information (generally)

- 3-Structural Information (mostly)
- 4-Quantitative information

What information do you need from the analysis ?

- 1-Low or High Mass range
- 2-Average or Monoisotopic mass (empirical)
- 3-Accurate Mass
- 4-Quantitation precision, accuracy, selectivity
- 4-Identification
- **5-Structural Information**
- 6-Isotope Ratios

Types of mass analyzer

Mass spectrometry is an analytic method that employs ionization and mass analysis of compounds to determine the mass, formula and structure of the compound being analyzed. A mass analyzer is the component of the mass spectrometer that takes ionized masses and separates them based on charge to mass ratios and outputs them to the detector where they are detected and later converted to a digital output.

There are six general types of mass analyzers that can be used for the separation of ions in a mass spectrometry.

1-Quadrupole Mass Analyzer.

- 2-Time of Flight Mass Analyzer.
- 3-Magnetic Sector Mass Analyzer.
- 4-Electrostatic Sector Mass Analyzer.
- 5-Quadrupole Ion Trap Mass Analyzers.
- 6-Ion Cyclotron Resonance.

Types of ionization techniques

- a- Volatile samples
- 1- Electron ionization (EI)
- 2- Chemical ionization(CI)
- b- Non-volatile samples
- 1- (FAB)Fast Atom Bombardment
- 2- Thermospray

3- (MALDI) Matrix Assisted Laser Desorption ionization

4- Electrospray ionization (ESI)

5- (APCI) Atmospheric Pressure Chemical ionization

It is important to understand two main categories that ionization falls under, hard and soft ionization:

a. <u>Hard ionization-</u> hard ionization evokes larger amounts of energy to the sample of interest in order to ionize the sample. Due to the larger amount of energy the bonds within the molecule tend to break more, resulting in an increase in fragmentation. Hard ionization techniques typically yield in a larger number of lower mass fragments as oppose to higher mass.

An example of this technique (EI method)

 b. <u>Soft ionization-</u> Soft ionization methods use smaller amounts of energy to ionize the sample, causing a decrease in fragmentation. This technique yields a larger amount of high mass fragments.

An example of this technique (Thermospray ,CI, APCI, FAB, ESI, and MALDI)

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