

techniques. The spectra give information on the fragmentation of molecules, characteristic of the structure.

The identification of known compounds is usually achieved by comparison of the measured spectrum with the spectrum of an authentic fully validated reference sample of the presumed compound, obtained under the same conditions; this comparison of spectra is now normally carried out by computerized search of a data base of stored reference spectra and direct computer-based comparison of the spectra.

The monitoring of known compounds can be carried out by using various techniques, the one selected for any one analysis being dependent on the sensitivity and selectivity required, the particular compound under study, the particular matrix of concern and the possible presence of other compounds. Selected ion monitoring (SIM) is a very selective technique especially when a high resolution instrument is used to monitor the effluent of the chromatograph. In specific reaction monitoring one or several fragmentation reactions of a selected molecule is monitored. Analytical limits can range from the picogram to the femtogram level, depending on the instrumental conditions used, which may include variations in the methods of ionising the sample.

The measurement of trace levels of known compounds can be carried out by the same techniques as used for the monitoring of known compounds.

As mentioned previously, mass spectrometers are now commonly interfaced with GC to give an extremely powerful integrated analytical system referred to as gas chromatography/mass spectrometry (GC-MS) in which the mass spectrum can be separately measured on each of the components separated from a mixture by the GC part of the integrated instrument. Considerable progress is now being made in the simplification of such integrated systems, with reduction in size, weight and cost. This principle of integrating a chromatographic separation technique with mass spectrometry is now being extended to include high performance liquid chromatography to give an integrated liquid chromatography/mass spectrometry (LC-MS) system. Although this has not yet progressed as far as with GC-MS the evolution of integrated LC-MS systems is likely to follow a similar route to GC-MS.