

APPLICATION OF MASS SPECTROMETRY FOR PESTICIDE ANALYSIS

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Mass Spectrometry has become a popular and essential analytical tool during the last decade especially with the introduction of atmospheric pressure ionization techniques such as electrospray ionization (ESI), atmospheric pressure chemical and photo ionization (APCI and APPI) techniques. Prior to that, samples were mostly analyzed by electron impact ionization technique which requires the sample to be volatile and thermally stable. Pure and electron impact stable compounds that are semi volatile could be analyzed by introducing the sample through direct insertion probe. Volatile mixtures are being analyzed by the gas chromatography-mass spectrometry (GC-MS) technique especially using capillary columns. Electron impact mass spectral library containing more than 6 million spectra are available with NIST and Wiley libraries. These data were generated using either magnetic sector or quadrupole mass spectrometers. Pesticides, insecticides, fungicides, herbicides, etc. can be grouped as volatile, semi volatile, and non-volatile compounds in general. Volatile compounds either in pure form or in a mixture are conveniently analyzed by GC-MS technique and identification can be done confidently with the help of the standard mass spectral libraries if data is available. Further confirmation of the molecular weight can be done by either positive

or negative chemical ionization (PCI or NCI) technique. Quantification at parts per billion level can be done by using multiple ion recording (MIR) technique. In recent times multiple reactions monitoring (MRM) technique is also being recommended under GC-MS conditions. As in the case of all the chromatography techniques, use of internal standards for reliable quantification is essential. Mass spectrometry has the advantage of using labelled analogues as internal standards so that the response factor becomes nearly one. Semi volatile and non volatile compounds can also be analyzed by GC-MS technique provided a stable volatile derivative can be quantitatively prepared. Otherwise, these compounds can be directly analyzed by liquid chromatography-mass spectrometry (LC-MS) technique. Unfortunately the ESI and APCI techniques only give only $[M+H]^+$ or $[M-H]^-$ ions under positive and negative modes respectively. Further limited structural information is obtained by MS-MS technique. Need based MS-MS libraries are being made for some group of compounds and that may be useful for identification of target compounds. However, for quantification purpose the MRM technique finds its superiority over other techniques mainly because majority of the pesticides are polar, samples can be analyzed with minimum clean up and at times even

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without HPLC. Instruments that can do 550 MRMs per second are available in the market. Only organo-chlorine pesticides are not amenable for LC-MS technique and hence, it is the method of choice for rapid and high throughput screening.

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