

**MULTIRESIDUE PESTICIDE SCREENING BY LC-ESI-TOF MS**Petra Decker<sup>2</sup>; Christian Neusuess<sup>3</sup>; Matthias Pelzing<sup>1</sup>

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Recently, bench-top Liquid Chromatography/Time-of-Flight Mass Spectrometry (LC/TOFMS) systems have become available that offer sufficient mass accuracy to be used in the routine screening of pesticides in different matrices.

LC/TOFMS offers significant advantages over conventional LC/MS and GC/MS techniques. LC/TOFMS can be used to measure the monoisotopic mass of pseudomolecular ions to within 3 mDa. A further tool for identification is the degree to which the isotopic pattern of a detected compound agrees with the theoretical pattern of any analyte (SigmaFit™). Results can be matched to a database containing the molecular formula of a large number of compounds and so provide a library search of similar breadth to that achieved with GC/MS spectral libraries. As with conventional LC/MS, LC/TOFMS can be used to detect thermo labile, polar, or high mass molecules unsuited to GC/MS.

A standard gradient LC with a 125x2.1mm Hypersil ODS C18 3µm column has been used applying an acetonitril/water gradient of 50min. An ESI-TOF mass spectrometer operated in positive ionization mode was used. External calibration with a calibrant injected at the beginning of each run allowed automated and non-interfering calibration with a mass accuracy better than 5ppm. The runs were automatically processed against a database consisting of name, elemental composition and retention time.

The ESI-TOF MS approach enables the screening for several hundred of possible pesticides within one run. The selectivity is based on the accurate mass, with mass traces defined within 0.003 Da over a dynamic range of about four orders of magnitude. Using a database of so far more than 340 pesticides spiked samples can be easily detected. Sensitivity in the range of low ppb range or even below can be achieved. Results for various matrices will be presented and discussed for potential need of sample preparation. An excellent linear range of 4 orders of magnitude is achieved, allowing the quantitation of the pesticides. In contrast to classical screening approaches by triple quadrupole instruments there are several benefits: 1. A high number of targets can be screened at the same time without loss of sensitivity 2. Unknown peaks can be identified based on accurate mass and true isotopic pattern 3. Data can be reprocessed later for additional compounds (archiving) 4. Profiling of the data allow for further statistical data evaluation. Benefits and requirements of the method will be discussed in detail.