

**THE USE OF ACCURATE MASS, ISOTOPE RATIOS AND MS/MS
FOR THE IDENTIFICATION OF PESTICIDES IN WATER**

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ABSTRACT: An algorithm for determining the presence of pesticides in different surface waters is presented. This algorithm profiles the accurate mass spectral data obtained using a quadrupole time-of-flight (QTOF) instrument, analyzing samples from different surface water sources. The accurate mass and isotopic ratios of those compounds found in each sample are compared to determine the similarities and distinctions among those samples. The compounds found are then fragmented to produce full scan MS/MS spectra for structural elucidation. The combination of this algorithm and the of the QTOF result in a very powerful technique for identifying large numbers of compounds.