

LC-TOFMS versus LC-MS/MS for multiresidue screening and quantitation of pesticides in fruits and vegetables

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Nowadays for non GC amenable compounds, liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS) is one of the most widely applied techniques to monitor a large number of pesticides in routine. In complex matrices, targeted analysis using selected reaction monitoring mode presents many advantages in terms of selectivity, sensitivity and quantification. However, with this approach, control laboratories must have at disposal large stocks of reference compounds to optimize MRM transitions for each substance. Financial investment for standards is very high and difficulties persist for not commercially available compounds such as metabolites or degradation products. Furthermore, according on the type of triple quadrupole used, the acquisition speed is now a bottleneck for the number of pesticides to monitor.

Liquid chromatography coupled to time-of-flight mass spectrometry (LC-TOFMS) was evaluated in our laboratory as a complementary technique for multiresidue screening and quantitation in fruits and vegetables samples. Indeed, compare to MSMS, TOFMS can produce accurate mass measurement at high resolution ($>12'000$ FWHM) allowing the generation of reconstructed ion chromatogram with narrow mass windows, thus providing good selectivity in complex sample matrices. Furthermore, accurate mass spectra measurement and correct isotope ratios are powerful data for identity confirmation of contaminants. The generic approach for analysis following by targeted data processing also give the opportunity to reprocess samples at any time to search for new analytes without further experiment. Last but not least, detection of known compounds based on molecular formula and exact mass chromatogram extraction are always possible even if the standard reference is not available.

UPLC-TOFMS was evaluated as an alternative to LC-MSMS for the screening and quantitative analysis of multiple pesticides residues in fresh fruits and vegetables after ethyl acetate extraction. Advantages, drawbacks and encountered difficulties with both techniques will be presented and discussed on the basis of real samples.