Development and Application of a Pesticide Library for the Identification and Confirmation Analysis in Various Sample Matrices by LC/MS/MS

Harald Möller-Santner, Applied Biosystems, Hamburg, Germany
André Schreiber, Applied Biosystems, Concord, ON, Canada *
Lutz Alder, Federal Institute for Risk Assessment, Berlin, Germany
* **Corresponding author - E-mail: andre.schreiber@lifetech.com; Phone: +1-905-660-9006;**

A new LC/MS/MS library containing more than 500 pesticides has been developed. Spectra were acquired using fast reversed phase LC coupled to a hybrid triple quadruple linear ion trap mass spectrometer. The MS/MS system was operated in Enhanced Product Ion scanning mode with standardized Collision Energy settings of 20, 35 and 50V and Collision Energy Spread of 35±15V. The acquisition and library search parameters have been optimized and then validated by library searching after injection of different dilutions and re-injection over a three months time period. Furthermore inter instrument repeatability was investigated.

Finally, the developed library was successfully used the screen food and drinking water samples for pesticides. A QuEChERS procedure was used to extract fruit and vegetable samples. Water was injected directly into the LC/MS/MS system. Multiple Reaction Monitoring (MRM) was used to screen for and quantify hundreds of targeted compounds. Traditionally the ratio of two MRM transitions is used for compound identification. However, the combination of selective and sensitive MRM detection and Enhanced Product Ion scanning with library searching allows screening for a larger panel of analytes and was able to reduce the number of false negative and false positive results. A similar experimental setup combining Enhanced MS with Enhanced Product Ion scanning can be used for General Unknown Screening. Further compound confirmation can be necessary using a different LC setup or GC analysis after extracting a second aliquot of the sample.

Keywords: pesticides, library, identification, comfirmation