The MasterView™ software allows quick processing and easy results review and reporting capabilities. Identification was based on retention time, accurate mass of the quasi-molecular ion, isotopic pattern TOF-MS and MS/MS information was used to identify and quantify targeted food residues. Quantitation was resolution and accurate mass data generated to get answers and results from these complex data.

Monitoring (MRM) mode. Single analysis because of their extra degree of selectivity and sensitivity when operated in Multiple Reaction Monitoring (MRM) mode.

LC-MS/MS is a powerful analytical tool for the analysis of food residues and contaminants. In particular, triple quadrupole based mass analyzers are popular for targeted quantitation of hundreds of food contaminants in a single analysis. The sensitivity of TripleTOF® 5600 system is comparable to the SCIEX QTRAP® 5500, respectively, operated in MRM mode, allowing extract dilution to minimize ion suppression while optimizing detection. The sensitivity of TripleTOF® 5600 System® Application Note SCIEX (2010) #0460110-02.

The results indicate that compounds with different MS/MS spectra are well detected. The authors thank Amadeo Fernandez-Alba (EURL) Almeria, Spain for providing EUPT samples.

**RESULTS**

**TOF/Q-TOF-MS Performance Characteristics**

Retention = 2.9 with signal / background ratio 500:1 and mass accuracy better than 0.5 ppm. These results are expected because of the excellent performance characteristics of the Sciex TOF-TOF®-MS system. The expected retention time of all target analytes was within ±0.5% of the measured values. Every compound entered the injection system as a single mass MS and MS/MS information was collected in a single injection on SCIEX TripleTOF® MS system. The sensitivity of TripleTOF®-MS based on the signal to background ratio was 0.3-0.5 and ion suppression was well below the required 5 ppm.

**Identification with high confidence is based on retention time matching, accurate mass and MS/MS library searching, to provide a high degree of confidence in assigning compound identity (4). MS/MS library searching, to provide a high degree of confidence in assigning compound identity (4) was well above the required 5 ppm. Compounds identified with high confidence were indicated using green check symbols. Sort the table by the fit factor column to display ID results from most confident to least confident.

**Screening**

**TopView® Software in MasterView™ Software**:

- Open data files, build up or open target IDSet, see and define concentration and threshold levels of analytes and control for quantitation.
- Set confidence settings and start processing. Result files and settings can be saved and loaded for reprocessing under different conditions.
- Extract SIM chromatograms and display MS and MS/MS spectra.
- Filter results based on identification criteria.
- Select results for reporting, export into a LIMS system, further processing in MultiQuant™ software, further processing in LibraryView™ software.

**Quantitation in MasterView™ Software**

**Automatic Identification of Known Chemical Residues and Contaminants in Food Samples using Accurate Mass LC-MS/MS Screening Techniques**

**MATERIALS AND METHODS**

- Fruit and vegetable samples from a local market were extracted with a 1:100: sample / acetone / methanol ratio (v/v) and loaded onto the autosampler.
- A novel approach of comparative multi-target screening to identify and quantify pesticide residues in food samples was applied to EUPT reference samples. The LC and chemical data were evaluated with Xcalibur™ software, version 2.0.7, and a SCIEX QTRAP® 5500 and TripleTOF® 5600 systems, respectively.
- The authors thank Amadeo Fernandez-Alba (EURL) Almeria, Spain for providing EUPT samples.

**Identification**

**MultiQuant™ software, identification with high confidence is based on retention time and accurate mass data generated to get answers and results from these complex data.**

**RESULTS**

**Table 1.** Results summary is listed in Table 1.

**CONCLUSIONS**

A novel approach of comparative multi-target screening to identify and quantify pesticide residues in food samples was applied to EUPT reference samples. The LC and chemical data were evaluated with Xcalibur™ software, version 2.0.7, and a SCIEX QTRAP® 5500 and TripleTOF® 5600 systems, respectively. The results were compared with the database files of the SCIEX QTRAP®® 5500 and SCIEX™ TripleTOF®® 5600 system.

**REFERENCES**

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**TRADMARKS/LICENSING**

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