**Food and Environmental**

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Confirmation of Contaminants in Water Using SCIEX Triple Quad™ 5500+ LC-MS/MS System − QTRAP® Ready and SCIEX OS-Q Software

Combining the Latest QTRAP Platform with Integrated Software for High Confidence ID Confirmation

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What: Testing labs are frequently confronted with the need for more confirmatory information when it comes to contaminant identification in environmental samples. In complex matrices, interferences may complicate interpretation of data resulting in false positives or reported residue levels to come into question. Combining speed and sensitivity with QTRAP technology and SCIEX OS-Q Software allows for the collection of full-scan MS/MS spectra for targeted anthropogenic pollutants in water samples. Those MS/MS data can be subsequently searched against SCIEX verified libraries for unambiguous qualitative confirmation of pesticide detection and ID.
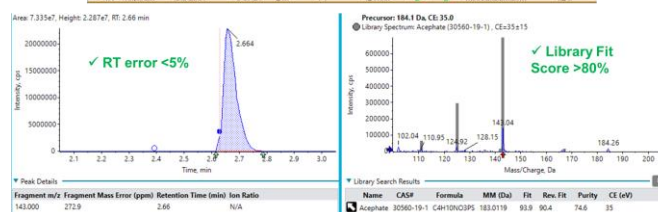
How: The MS method was set up with a targeted list of PPCPs and pesticides comprising over 200 MRM transitions. IDA (Information Dependent Acquisition) criteria were defined such that Enhanced Product Ion (EPI) acquisition would be triggered when an MRM signal exceeded a threshold of 2000 cps. This type of data acquisition results in the collection of MS/MS spectral information in addition to the MRM signal (Figure 1).
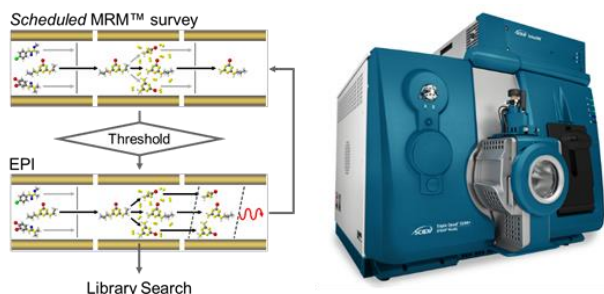
Figure 1. The SCIEX Triple Quad 5500+ System – QTRAP Ready for MRM-MS/MS. The QTRAP system functionality was employed with EPI scan type triggered by signal from target pesticides monitored in MRM mode. The resulting MS/MS spectrum were matched to library spectra for confirmation.

Samples of surface water were collected from the environment and analyzed. Data were processed in SCIEX OS-Q Software for quantitation by MRM and spectral identification by library matching. Figure 2 shows MS/MS spectra being used to confirm the identity of Acephate by both MS/MS and Retention Time. This additional stringency in identity confirmation could help protect against reporting false positives and provide additional, defensible confidence in the qualitative and quantitative results.

Figure 2. High Confidence in Positive Detection Possible with MS/MS and SCIEX OS-Q Software. ID and quantitation of contaminants can be achieved with high confidence using the ion trap to collect MS/MS spectra in addition to MRM peaks. Retention time plus MS/MS spectra provide confirmation that the identified peak is Acephate. SCIEX OS-Q Software results table utilizes visual features (green check marks) in the Confidence columns where peaks have been confirmed with library fit score of >80%. The Confidence columns are filterable and sortable to find positive matches or potentially matches quickly, making rapid assessment of large sample sets possible, ultimately resulting in greater data processing efficiency and increased qualitative confidence in reported detects during results reporting for residues in water samples.