

November 5, 2026 (14:45-15:30)



VENDOR SEMINAR:

From weighed sample to final report: An automated QuPPE workflow combining robotic sample preparation, LC-MS/MS and Python-based evaluation

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Highly polar pesticides and their metabolites are important target compounds in food control, but they are not adequately covered by conventional QuEChERS-based multiresidue methods. The Quick Polar Pesticides method (QuPPE) provides a dedicated LC-MS/MS-based approach for these analytes; however, its routine implementation still involves several manual steps in sample preparation, instrumental sequence handling, data evaluation and reporting.

This contribution presents a workflow for QuPPE-based analysis in which robotic sample preparation, LC-MS/MS measurement and Python-based data evaluation are connected into a largely continuous process. Starting from the weighed sample, a laboratory robot integrated with the analytical system performs the addition of isotope-labelled internal standards and extraction solvent, extraction by shaking, centrifugation and transfer of the supernatant into the analytical workflow. The prepared extracts are then measured by LC-MS/MS using QuPPE-compatible chromatographic and mass spectrometric conditions.

A key aspect of the workflow is the direct integration of the laboratory robot with the LC-MS/MS system. Sample preparation and measurement are organized as one continuous process: samples are prepared by the robot and transferred directly into the analytical sequence, reducing intermediate handling steps and supporting consistent timing between extraction, centrifugation, transfer and measurement. This setup is particularly relevant for routine QuPPE analysis, where reproducibility, traceability and controlled processing conditions are essential.

The analytical data are evaluated using a Python-based script that supports automated review and structured reporting. The script processes batch information and analytical results, checks predefined quality criteria such as calibration performance, internal standard response, retention time stability, ion ratio agreement and blank values, calculates concentrations and flags results requiring manual review. This creates a transparent data pathway from measurement to report while maintaining expert control over final result assessment.

The automated workflow is validated according to the relevant SANTE criteria for pesticide residue analysis. Method performance is assessed in terms of selectivity, linearity, recovery, repeatability, within-laboratory reproducibility and limits of quantification. In addition, the applicability and trueness of the workflow are verified using suitable reference material.

The presentation includes the handling of methanol-based extracts, timing and reproducibility of extraction and centrifugation steps, integration of quality-control samples, prevention of carry-over and contamination, traceability of processing steps and the balance between automated evaluation and expert review. Particular attention is given to the question of which parts of the QuPPE workflow can be reliably automated and where laboratory-specific control points remain necessary.

Using QuPPE analysis as an example, the workflow illustrates how direct robot-LC-MS/MS integration and automated data evaluation can support standardization, documentation and reproducibility in routine food control laboratories. The aim is not to replace analytical expertise, but to reduce repetitive manual operations and create a transparent process from sample preparation to final report.