Using the iDQuant™ Standards Kit for Pesticide Analysis to Analyze Residues in Fruits and Vegetable Samples

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Overview

The iDQuant™ Standards Kit for Pesticide Analysis of certified reference material (ISP Guide 34, IOS/IEC 17025 and ISO 9001:2008) includes 204 pesticides. This kit has been designed to eliminate the need to source pesticides individually, and measure each one manually. This allows to setup, verify, and validate the performance of your pesticide screening method faster.

Here we present example data where we used the iDQuant™ Kit to screen for, quantify, and identify pesticides in extracts of fruits and vegetables using Liquid Chromatography tandem Mass Spectrometry (LC-MS/MS) with an AB SCIEX QTRAP® 5500 system.

Introduction

Many recent developments such as generic extraction procedures, (like QuEChERS), generic LC separation methods, and highly selective and sensitive MS/MS detectors have established LC-MS/MS as a standard technique for the analysis of pesticide residues in food. Hundreds of targeted analytes can be detected in a single analytical run. Software designed for ease-of-use like Cliquid® software in conjunction with iMethod™ applications made the fast adaptation of LC-MS/MS in new routine testing laboratories possible. For a while, data processing was the bottleneck for most laboratories, but the development of fast and automatic data processing and reporting tools sped up the delivery of analytical results.

A major hurdle for each laboratory is method setup, verification, and validation. The newly available iDQuant™ kit can be used for the following tasks:

- Tune or verify MRM transitions for best selectivity and sensitivity of MS/MS detection
- Measure retention times to quickly update acquisition methods using the Scheduled MRM™ algorithm
- Verify the performance of LC methods
- Investigate recovery and reproducibility of sample preparation procedures
- Validate the performance of the complete method procedure

Description of the iDQuant™ Standards Kit for Pesticide Analysis

Content

The iDQuant™ Kit contains a total of 204 pesticides in 10 mixes at a concentration of 100 μg/mL and a certificate of analysis for each mixture. The pesticides are listed in Table 1.
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Storage and Stability

The pesticides of the iDQuant™ Kit are stable in the sealed ampoules for one year at -20°C. An example of stability test results is shown in Figure 2.

Stock solutions of the 204 pesticides at 1 μg/kg can be simply prepared by mixing 10 μL of each mix and diluting with 900 μL of acetonitrile. It is recommended to store aliquots of this stock solution in amber glass vials at -20°C, for future use.

Calibration standards can be prepared by serial dilution of the prepared stock solutions using water or the aqueous mobile phase of the LC system. It is recommended to prepare calibration standards daily to avoid degradation of pesticides.

LC-MS/MS Method Setup

The iMethod™ application for pesticide screening contains a ready-to-use method to screen for all 204 pesticides of the iDQuant™ kit.

The kit can also be used to fine tune MRM conditions or to adjust retention times of existing methods to update the Scheduled MRM™ algorithm for best performance (Figure 3).

Application of the iDQuant™ Standards Kit for Pesticide Analysis

Experimental

- The iDQuant™ standards kit for pesticide analysis was used for method setup and preparation of calibration standards.

- Fruit and vegetable samples were extracted using a QuEChERS procedure and diluted 10x with water to optimize chromatographic peak shape and minimize possible matrix effects and interferences.

- LC separation was achieved on a Shimadzu UFLCXR system with a Restek Ultra Aqueous C18 3 µm (100x2.1 mm) column and a 15 min gradient of water and methanol with ammonium formate buffer at a flow rate of 0.5 mL/min. The injection volume was set to 10 μL.

- The AB SCIEX QTRAP® 5500 system was operated with Turbo V™ source and Electrospray Ionization (ESI) probe. 436 MRM transitions were monitored using the Scheduled MRM™ algorithm with a detection window of 120 s and a target scan time of 0.7 s.

- MultiQuant™ 2.0.2 software with the ‘Multicomponent’ query was used for quantitative data processing (Figure 4).
Table 2. Pesticides quantified in fruit and vegetable samples above 10 μg/kg and positively identified using their retention time and MRM ratio

<table>
<thead>
<tr>
<th>Sample</th>
<th>Pesticide</th>
<th>Concentration (μg/kg)</th>
<th>Retention time (min)</th>
<th>Expected retention time (min)</th>
<th>MRM ratio</th>
<th>Expected MRM ratio</th>
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* Dimethomorph in the grapes sample after washing was quantified and identified below 10 μg/kg
Results

All identified and quantified pesticides are listed in Table 2. The 'Multicomponent' query was used in MultiQuant™ software to automatically report concentrations above the threshold of 10 μg/kg and to compare MRM ratios for compound identification. The maximum permitted tolerances for MRM intensities of the SANCO guideline ‘Method validation and quality control procedures for pesticide residue analysis in food and feed’ were used for identification. As part of the samples set grapes were analyzed with and without washing before extraction. Half of the grapes were simply rinsed under running tap water for approximately 30 seconds.

Summary

The results in Table 2 show that this washing method is not sufficient to completely remove fungicide before consumption.

References

3 SANCO/10684/2009