

# Food and Environmental Application Compendium

7250 GC/Q-TOF



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## 7250 GC/Q-TOF

The Agilent 7250 GC/Q-TOF system delivers full-spectrum, high-resolution, accurate mass data with a wide dynamic range for identifying and quantifying GC-amenable compounds. This high-resolution GC/Q-TOF enables accurate mass screening by GC/MS and enhanced compound identification through MS/MS, low-energy electron ionization, and complimentary chemical ionization techniques.

Whether it is used in complex metabolomics studies, pesticide screening in challenging matrices, or compound identification in herbal extracts, quadrupole time-of-flight GC/MS provides the ultimate in performance. Designed for real-world analysis and built for laboratory robustness, this accurate mass screening GC/MS delivers consistent confidence in results, allowing you to see the whole picture.



# 7250 GC/Q-TOF Application Notes

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Agriculture

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## Workflow for Food Classification and Authenticity using Yerba Mate and High-Resolution GC/Q-TOF



**Author**  
Sofia Nieto and  
Melissa Churley  
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**Abstract**  
This application note provides an example of a novel food authenticity workflow that can be used for food classification and detection of food fraud. Different brands of yerba mate, a South American herbal tea, were used to illustrate the workflow. The food authenticity workflow described here takes advantage of high-resolution accurate mass GC/Q-TOF data, as well as differential analysis software that enables routine screening of food samples.

## Workflow for Food Classification and Authenticity using Yerba Mate and High-Resolution GC/Q-TOF

This application note provides an example of a novel food authenticity workflow that can be used for food classification and detection of food fraud. Different brands of yerba mate, a South American herbal tea, were used to illustrate the workflow. The food authenticity workflow described here takes advantage of high-resolution accurate mass GC/Q-TOF data, as well as differential analysis software that enables routine screening of food samples.

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## Black Pepper Authenticity Workflow Using the High-Resolution Agilent 7250 GC/Q-TOF

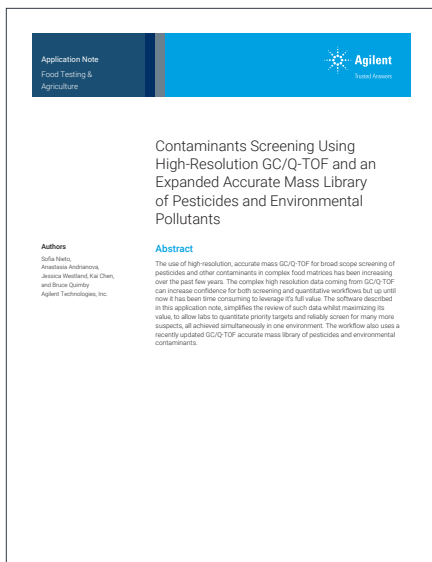
**Author**  
Sofia Nieto and  
Melissa Churley  
Agilent Technologies, Inc.

**Abstract**  
Black pepper is a highly valued commodity known to be subject to economically motivated adulteration.<sup>1</sup> This application note discusses a novel food authenticity workflow targeted for routine analysis that allows to distinguish black pepper samples from different geographic regions and detect adulteration. The workflow uses high-resolution mass spectrometry (HRMS) with Agilent Mass Profiler Professional (MPP) and Agilent MassHunter Classifier software to build and apply the classification model.

## Black Pepper Authenticity Workflow Using the High Resolution Agilent 7250 GC/Q-TOF

Black pepper is a highly valued commodity known to be subject to economically motivated adulteration.<sup>1</sup> This application note discusses a novel food authenticity workflow targeted for routine analysis that allows to distinguish black pepper samples from different geographic regions and detect adulteration. The workflow uses high-resolution mass spectrometry (HRMS) with Agilent Mass Profiler Professional (MPP) and Agilent MassHunter Classifier software to build and apply the classification model.

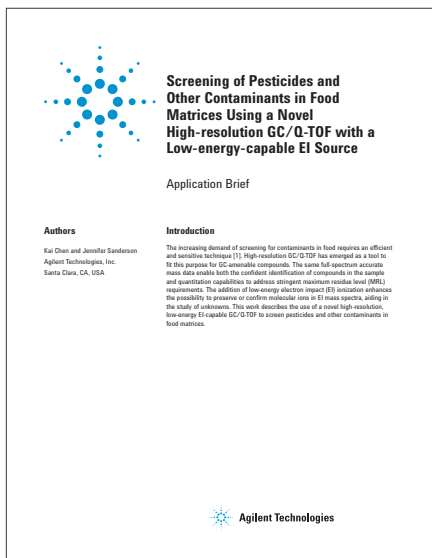
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## Contaminants Screening Using High-Resolution GC/Q-TOF and Expanded Accurate-Mass Library of Pesticides and Environmental Pollutants

The use of high-resolution, accurate mass GC/Q-TOF for broad scope screening of pesticides and other contaminants in complex food matrices has been increasing over the past few years. The complex high resolution data coming from GC/QTOF can increase confidence for both screening and quantitative workflows but up until now it has been time consuming to leverage its full value. The software described in this application note, simplifies the review of such data whilst maximizing its value, to allow labs to quantitate priority targets and reliably screen for many more suspects, all achieved simultaneously in one environment. The workflow also uses a recently updated GC/Q-TOF accurate mass library of pesticides and environmental contaminants.

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## Screening of Pesticides and Other Contaminants in Food Matrices Using a Novel High-resolution GC/Q-TOF with a Low-energy-capable EI Source

This work describes the use of a novel high-resolution, lowenergy Elcapable GC/Q-TOF to screen pesticides and othThe increasing demand of screening for contaminants in food requires an efficient and sensitive technique [1]. High-resolution GC/Q-TOF has emerged as a tool to fit this purpose for GC-amenable compounds. The same full-spectrum accurate mass data enable both the confident identification of compounds in the sample and quantitation capabilities to address stringent maximum residue level (MRL) requirements. The addition of low-energy electron impact (EI) ionization enhances the possibility to preserve or confirm molecular ions in EI mass spectra, aiding in the study of unknowns. This work describes the use of a novel high-resolution, low-energy EI-capable GC/Q-TOF to screen pesticides and other contaminants in food matrices.

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## Short Chain Chlorinated Paraffins (SCCP) Analysis Using Negative Chemical Ionization (CI) and Low Energy EI by High-Resolution 7250 GC/Q-TOF

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**Abstract**  
The Agilent 7250 Series high-resolution accurate mass GC/Q-TOF was used to analyze one of the most challenging group of compounds, short chain chlorinated paraffins (SCCPs), using a comprehensive approach including both negative chemical ionization (NCI) as well as low energy electron ionization (LE-EI). The current study focuses on evaluating the suitability of the LE-EI and NCI modes of the Agilent GC/Q-TOF for the SCCP analysis, and reveals the advantages of each technique.

## Short Chain Chlorinated Paraffins (SCCP) Analysis Using Negative Chemical Ionization (CI) and Low Energy EI by High-Resolution 7250 GC/Q-TOF

The Agilent 7250 Series high-resolution accurate mass GC/Q-TOF was used to analyze one of the most challenging group of compounds, short chain chlorinated paraffins (SCCPs), using a comprehensive approach including both negative chemical ionization (NCI) as well as low energy electron ionization (LE-EI). The current study focuses on evaluating the suitability of the LE-EI and NCI modes of the Agilent GC/Q-TOF for the SCCP analysis, and reveals the advantages of each technique.

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## Analysis of Wastewater Effluent Samples to Identify Toxic Chemicals Using the High-Resolution Agilent 7250 GC/Q-TOF

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**Abstract**  
This study used a workflow for broad scope suspect screening to identify toxic chemicals in wastewater effluents. The comprehensive approach combined targeted and untargeted methods using a high-resolution accurate mass Agilent 7250 GC/Q-TOF in multiple ionization modes, the GC/Q-TOF screening workflow in Agilent MassHunter Quantitative Analysis software 10.1, and the GC/Q-TOF accurate mass library of pesticides and environmental contaminants.

## Analysis of Wastewater Effluent Samples to Identify Toxic Chemicals Using the High-Resolution Agilent 7250 GC/Q-TOF

This study used a workflow for broad scope suspect screening to identify toxic chemicals in wastewater effluents. The comprehensive approach combined targeted and untargeted methods using a high-resolution accurate mass Agilent 7250 GC/Q-TOF in multiple ionization modes, the GC/Q-TOF screening workflow in Agilent MassHunter Quantitative Analysis software 10.1, and the GC/Q-TOF accurate mass library of pesticides and environmental contaminants.

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### Comprehensive Profiling of Environmental Contaminants in Surface Water Using High-Resolution GC/Q-TOF

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**Abstract**  
Monitoring of environmental pollutants in surface water is a challenging task due to large number of contaminants, continuous change of their relevance in the environment, and toxicity at low concentration (for example, for pyrethroids and some organophosphate pesticides) requiring methods with low detection limits. The use of accurate mass high-resolution MS (HRMS) techniques to characterize known and unknown pollutants in a sample is gaining in popularity. However, several environmental contaminants are low molecular weight, volatile, or nonpolar, making them much more amenable to analysis by GC rather than LC. Therefore, to achieve high sensitivity together with an expanded analysis scope, a comprehensive workflow including targeted quantitation, suspect screening, and a nontargeted approach with a high-resolution accurate mass GC/Q-TOF was applied to screen for environmental pollutants in water samples.

## Comprehensive Profiling of Environmental Contaminants in Surface Water Using High-Resolution GC/Q-TOF

Monitoring of environmental pollutants in surface water is a challenging task due to large number of contaminants, continuous change of their relevance in the environment, and toxicity at low concentration (for example, for pyrethroids and some organophosphate pesticides) requiring methods with low detection limits.<sup>1</sup> The use of accurate mass high-resolution MS (HRMS) techniques to characterize known and unknown pollutants in a sample is gaining in popularity. However, several environmental contaminants are low molecular weight, volatile, or nonpolar, making them much more amenable to analysis by GC rather than LC. Therefore, to achieve high sensitivity together with an expanded analysis scope, a comprehensive workflow including targeted quantitation, suspect screening, and a nontargeted approach with a high-resolution accurate mass GC/Q-TOF was applied to screen for environmental pollutants in water samples.

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© Agilent Technologies, Inc. 2021  
Published in the USA, November 4, 2021  
5994-4294EN