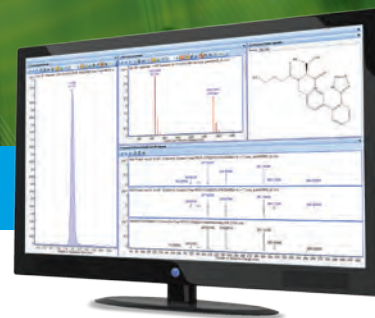# SIMPLIFY YOUR COMPREHENSIVE PESTICIDES SCREENING

Agilent Pesticide LC/MS Personal Compound Database and Library

To meet stringent regulatory standards for pesticides, labs must be able to detect and identify more than 1,000 pesticides.

Conventional, multi-target pesticide screening methods are based upon highly sensitive triple quadrupole technology which excels at targeted analysis of a defined set of compounds. But choosing which pesticides to test is a growing challenge. As a result, many labs are now harnessing the power of untargeted, full-spectrum mass spectrometry (MS) to also investigate compounds beyond the scope of targeted methods.

Confidently use accurate mass to perform target and suspect screening

You can screen for more than 1,700 pesticides—and confidently identify compounds by comparing accurate mass spectra—when you combine TOF or Q-TOF LC/MS with the Agilent Pesticide Personal Compound Database and Library (PCDL).

In addition, All Ions MS/MS acquisition allows you to perform retrospective analysis by measuring precursor ions and fragments for a virtually unlimited number of compounds. That means you can re-analyze or mine the data at any time—without reruns—to investigate samples for emerging contaminants.

The following components are included in the Agilent Pesticide PCDL—saving you time and maximizing performance

- Curated accurate-mass database with more than 1,700 compounds
- Accurate-mass MS/MS spectra for more than 800 compounds—over 2,700 spectra total
- Searchable user notes containing compound class and regulation tags
- Includes Chinese/Japanese names
- Quick-start guide with data examples and familiarization exercises
- Method Setup Guide that shows you how to create acquisition methods
- Application notes with detailed LC/MS method parameters
- Latest version of PCDL Manager Software
- Free database upgrades for 3 years

Agilent Technologies

PERFORM TRULY COMPREHENSIVE SCREENING FOR AN UNLIMITED NUMBER OF COMPOUNDS

Combining the Agilent Pesticide PCDL with the accurate mass capabilities of LC/TOF and Q-TOF instruments enables you to:

- **Acquire full-spectrum, untargeted data** using All Ions MS/MS

- **Identify compounds** through accurate mass, retention time, isotope pattern, and fragment confirmation

- **Perform presumptive matching** of acquired and library spectra—without the need to source standards

- **Create a custom PCDL** for more focused screening

- **Propose a suspect list** based on MS data and the "Find by Formula" algorithm

- **Confirm contaminants and eliminate false positives** with targeted MS/MS and library search

- **Mine data from Auto MS/MS experiments** using "Molecular Feature Extraction," and search for proposed compounds against the PCDL

- **Add your own compounds and library spectra** to create PCDLs specific to your needs

- **Perform retrospective data analysis** using newly added PCDL compounds—without the need to re-run samples

Simply put, the Pesticide PCDL makes compound confirmation and data mining easier, even for high-throughput labs.
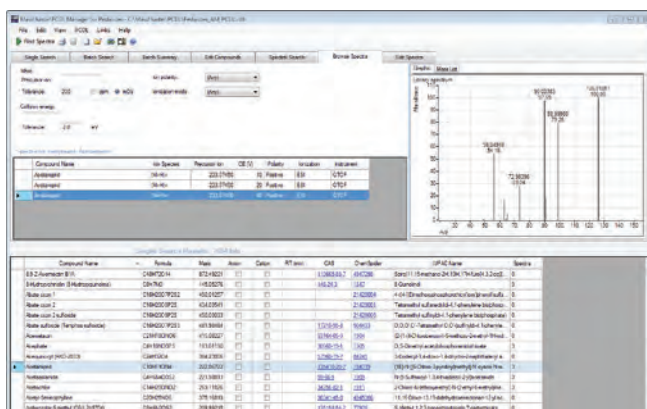

Straightforward data mining and unambiguous identification using All Ions Software.

Top: Auto MS/MS spectrum

Middle: Mirror spectrum

Bottom: Library spectrum

Reliably confirm compounds by library matching using Auto MS/MS.

PCDL Manager Software makes it easy to control the database and library.

PROTECT OUR FOOD SUPPLIES
AND COMPLY WITH REGULATORY STANDARDS

The Agilent Pesticide PCDL can help you meet the strict requirements established by global food regulatory agencies, including the following:

EU
EC 396/2005, EU WFD

U.S.
40 CFR part 180, EPA 535/1699, Draft CCL4

China/Japan
GB 2763-2014, NY 235, JPL, JDWQS

Available class tags
Pesticides, insecticides, herbicides, fungicides, etc.

Maximize your data quality with database and library curation

- Compound common name and IUPAC name
- Accurate mass of neutral molecule
- Molecular formula and structure
- Ion type (anion, cation, or neutral)
- CAS number/PubChem link (if existing)
- ChemSpider ID and hyperlink (if existing)
- Precursor and product ion peaks corrected to theoretical accurate mass
- Spectra acquired at 10, 20, and 40 V collision energy
- Includes adduct & loss spectra
- Spectra measured in positive and/or negative ion mode, where applicable
- Spectra filtered for signal intensity and curated for spectrum noise, chemical impurities, and incorrectly set instrument parameters

Application consulting lets you focus on what you do best

Installation and familiarization (optional):

Experienced service personnel will install the PCDL, verify all functions with an Agilent checkout sample, and familiarize you with the supporting software.

Advanced application consulting (optional):

Let us help you get the most out of your PCDL by setting up screening methods for your samples of interest.

Learn how to analyze more pesticides, faster.
Visit **www.agilent.com/chem/application-kits**

Complete your pesticides analysis workflow

MassHunter data acquisition and analysis software

Quickly implement high-quality screening methods, and modify these methods to meet your future needs. You can also customize your PCDL to suit your application.

Agilent 1290 Infinity II LC system

Achieve unmatched chromatographic resolution and reduced runtimes, and produce the high-quality data you need for sensitive, reproducible screening.

Agilent TOF and Q-TOF LC/MS systems

The full-scan capability of All Ions MS/MS lets you access all the data, all the time, so you can screen for large numbers of suspect and unknown pesticides using accurate mass. What's more, the Agilent Jet Stream electrospray ion source dramatically lowers your detection limits.

Agilent LC columns, supplies, and sample prep products

Increase your uptime and achieve the best scientific outcomes.

Ordering Information:

Pesticide Personal Compound Database and Library (G3878CA)
Required but not included with the Pesticide PCDL:
Agilent 1260 or 1290 Infinity II LC
Agilent 6200 Series TOF or 6500 Series Q-TOF LC/MS
Agilent MassHunter Acquisition Software (B.05 or higher) and Windows 7 (64-Bit)
Agilent MassHunter Qualitative Analysis Software (B.07 SP1 or higher)
Agilent MassHunter Quantitative Analysis Software (B.07 or higher)
OPTIONAL: G3878CA #001 Installation and Familiarization Service
OPTIONAL: Advanced Application Consulting H2149A (Americas); R1736A (other regions)

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For a description of available LC/MS Databases and Libraries, and GC/MS Analyzers, visit
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