SIMPLIFY YOUR SCREENING OF WATER CONTAMINANTS

The Measure of Confidence

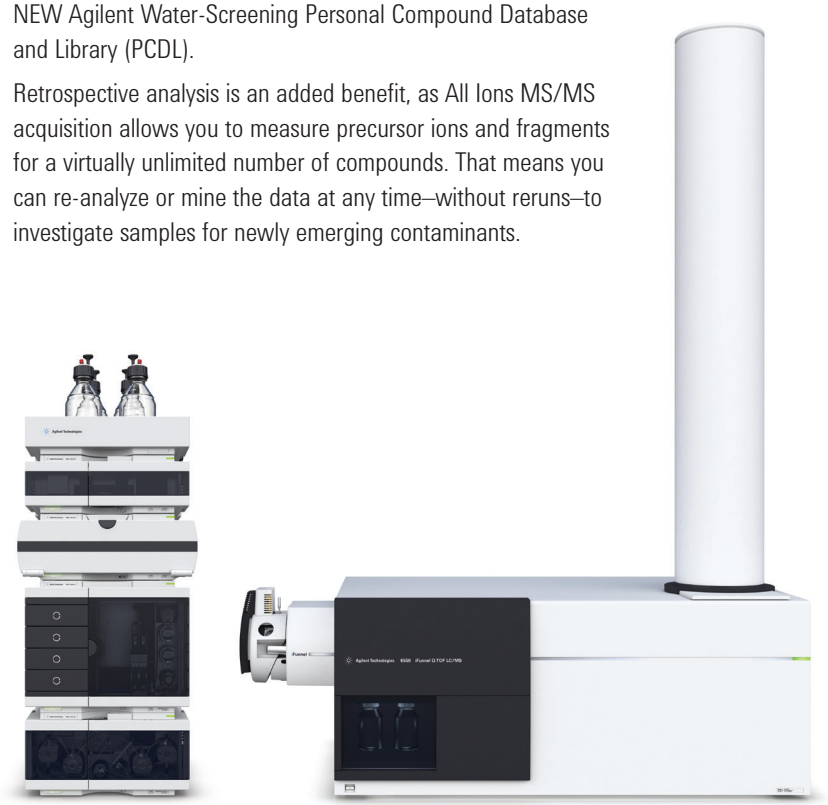
Agilent Water-Screening LC/MS Personal Compound Database and Library

Confidently perform target and suspect screening using accurate mass

Demand for comprehensive water-screening methods continues to grow, driven by new regulations and increasing interest in contaminants of emerging concern–such as pharmaceuticals and personal-care products (PPCPs).

You can screen for more than 1,400 water contaminants with highly confident identification using accurate mass MS/MS spectra, by combining TOF or Q-TOF LC/MS instruments with the NEW Agilent Water-Screening Personal Compound Database and Library (PCDL).

Retrospective analysis is an added benefit, as All Ions MS/MS acquisition allows you to measure 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 newly emerging contaminants.



The PCDL includes the following components that save time and maximize performance:

- Curated accurate-mass database with more than 1,400 compounds
- Searchable user notes containing compound class and regulation tags
- Chinese names for over 500 compounds and Japanese names for over 250 compounds
- Accurate-mass MS/MS spectra for more than 1,000 compounds
- Retention times for over 260 compounds
- Quick-start guide with data examples and familiarization exercises
- Application note with detailed LC/MS method information
- Latest version of PCDL Manager Software

Agilent Technologies

Target and suspect screening workflows with the PCDL

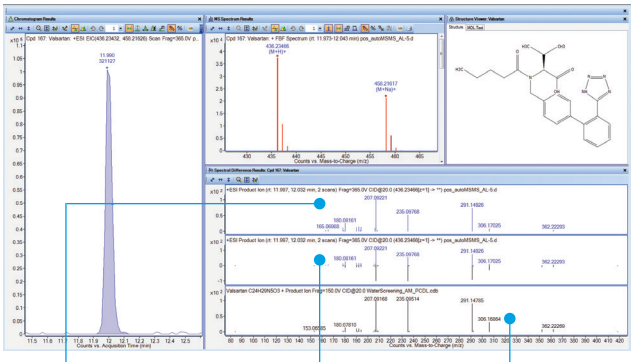
The Agilent Water-Screening PCDL, combined with the accurate mass capabilities of LC/TOF and Q-TOF instruments, enables you to:

- Acquire full-spectrum, untargeted data using All Ions MS/MS and identify compounds through accurate mass, retention time, isotope pattern, and fragment confirmation
- Perform presumptive matching of acquired spectra with library spectra–without the need to source standards
- Retention times add another degree of identification confidence and help avoid false positives
- Create a custom PCDL for a more focused screening approach
- Propose a suspect list with MS data and the "Find by Formula" algorithm, then confirm contaminant presence 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 unique compounds and library spectra to create PCDLs specific to your analysis
- Perform retrospective analysis of data with compounds newly added to the PCDL, without a need to re-run samples

The NEW Water-Screening PCDL makes compound confirmation and data mining easier–even for high-volume labs–to perform truly comprehensive screening of an unlimited number of compounds.

Easy data mining and unambiguous identification using All Ions Software

Attain compound confirmation by library matching using Auto MS/MS

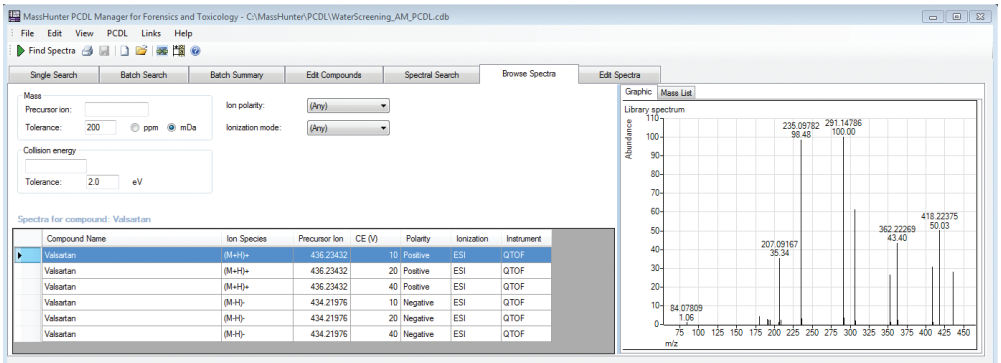


Top: Auto MS/MS spectrum

Middle: Mirror spectrum

Bottom: Library spectrum

PCDL Manager Software provides easy management of the database and library



Protect our water supply and comply with regulatory standards

The Agilent Water-Screening PCDL can help you meet the strict requirements established by global compliance agencies. It includes more than 1,400 compounds–including those specified by the following regulations and lists:

EU regulations

Priority compounds from the EU water framework directive

U.S. regulations

Environmental Protection Agency methods 521, 535, 539, 1694, 1698, 1699, and Draft CCL4

Chinese regulations and lists

- CN-EPA screening list
- CN-NY methods 193, 235, 265, 560
- CN-CDC survey list
- CN-antibiotics list
- CN-GB 2763-2014

Japanese regulations and lists

- Japan positive list
- JDWQS

Available class tags

PPCPs, pesticides, veterinary drugs, human drugs, polar metabolites, cyanotoxins, and class tags for all regulations and lists above

Database and library curation assure highest data quality

Each curated database entry includes:

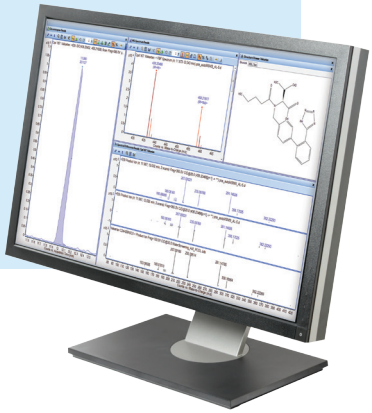
- Compound common name
- Accurate mass of neutral molecule
- IUPAC name
- Molecular formula
- Molecular structure
- Ion type (Anion, Cation, or Neutral)
- CAS number/PubChem link (if existing)
- ChemSpider ID and hyperlink (if existing)

Accurate mass spectral library curation:

- Each precursor and product ion peak corrected to theoretical accurate mass
- Spectra acquired at 10, 20, and 40eV Collision Energy
- Spectra measured in positive and/or negative ion mode where applicable
- Spectra are filtered for signal intensity and curated for:
  - Spectrum noise
  - Chemical impurities
  - Incorrectly set instrumentation parameters

Complete your water analysis workflow with leading-edge solutions from Agilent

- **MassHunter data acquisition and analysis software** lets you quickly implement high-quality screening methods, which you can modify to meet your future needs. You can also customize your PCDL.
- **The Agilent 1290 Infinity II LC system** provides unmatched chromatographic resolution and reduced runtimes, delivering the high-quality data you need for sensitive and reproducible screening applications. What's more, the Agilent Jet Stream electrospray ion source dramatically lowers detection limits for emerging contaminants in water.
- **Agilent TOF and Q-TOF LC/MS systems** give you reliable MS and MS/MS mass accuracy. 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 analytes and unknown contaminants.
- **Best-in-class application consulting** plus a large portfolio of sample-prep products, LC column phases, and other consumables–increases productivity and helps you focus on what *you* do best.



Ordering Information:

Agilent Water-Screening Personal Compound Database and Library (G6882CA)

The following are required, but not included, with the Water-Screening PCDL:

- Agilent 6200 Series TOF or 6500 Series Q-TOF LC/MS systems
- 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)

To learn more about the Agilent Water-Screening PCDL, visit **www.agilent.com/chem/waterscreening**

Put your lab on the productivity fast track.

Contact your local Agilent Representative or Agilent Authorized Distributor at **www.agilent.com/chem/contactus**

Or call **800-227-9770** (in the U.S. or Canada)

Visit **www.agilent.com/chem/ms** for a description of available Analyzers and Application Kits

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