

# SIMPLIFY YOUR COMPREHENSIVE EXTRACTABLES AND LEACHABLES SCREENING



## Agilent Extractables and Leachables LC/MS PCDL



Manufacturers of pharmaceuticals, drug packaging components, medical devices, and packaged food products have come under growing pressure to perform sensitive and accurate analytical studies on extractable and leachable (E&L) compounds.

Agilent offers a full range of complementary techniques and software tools for the analysis of small and large molecule E&Ls (volatiles, semi-volatiles, non-volatiles, heavy metals, and oligomers).

### Confidently use accurate mass to perform target and suspect screening

Search for more than 1,000 extractables and leachables—confidently identifying compounds from accurate mass spectral data obtained from LC/MS TOF or Q-TOF and the Agilent Extractables and Leachables Personal Compound Database and Library (PCDL).

In addition, perform retrospective analysis for a virtually unlimited number of compounds based on All Ions MS/MS acquisition. You can re-analyze or mine the data at any time—without reruns—to investigate samples for new extractable/leachable compounds.

### The following are included in the Agilent Extractables and Leachables PCDL—saving you time and maximizing performance

- Curated accurate-mass database with more than 1,000 compounds
- Accurate-mass MS/MS spectra for 360 compounds—over 1,300 spectra total
- Searchable user notes containing compound class and regulation tags
- Retention time information added to more than 125 compounds
- Chinese names
- Quick-start guide with data examples and familiarization exercises
- Latest version of PCDL Manager Software
- Free database upgrades for 3 years



**Agilent Technologies**

# PERFORM TRULY COMPREHENSIVE SCREENING FOR AN UNLIMITED NUMBER OF COMPOUNDS

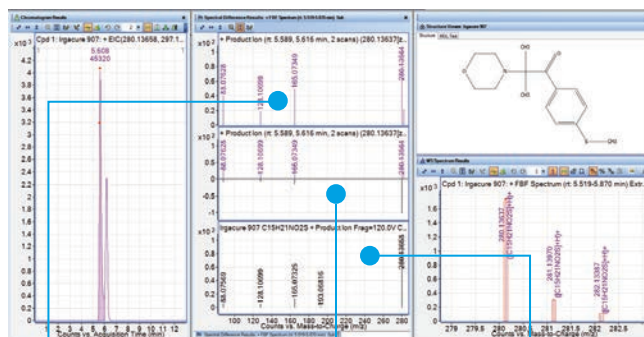
Combining the Agilent Extractables and Leachables PCDL with the accurate mass capabilities of LC/TOF and Q-TOF instruments enables you to:

- **Acquire full-spectrum, untargeted data** using multiple data acquisition modes such as MS only and 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 MS only and Auto MS/MS experiments using “Molecular Feature Extraction” or “Profiler,” and search for proposed compounds against the PCDL
- **Identify differences** between two or multiple groups of samples using either Mass Profiler or Mass Profiler Professional software with the combination of formula generation and database searching for identification
- **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 Extractables and Leachables PCDL makes compound confirmation and data mining easier for high-throughput labs and labs new to LC/MS alike.

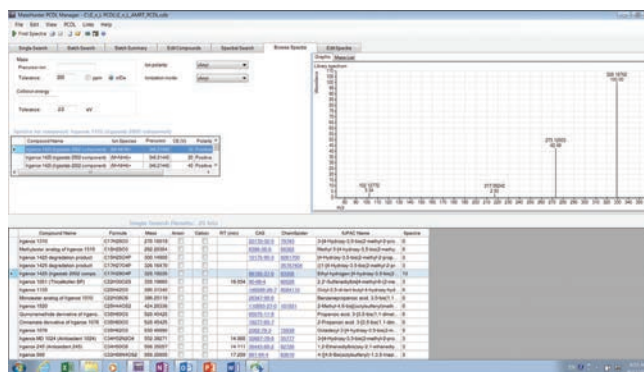


Straightforward data mining and unambiguous identification using All Ions Software.



**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.

# BE PREPARED FOR THE GROWING REQUIREMENTS OF EXTRACTABLES AND LEACHABLES ANALYSIS

Compound class and regulation tags in the Agilent Extractables and Leachables PCDL allow you to easily narrow down your screening applications:

- SWISS Ordinance (SR 817.023.21), (EC) No. 1272/2008 and EU 2005/84/EC
- ELSIE (The Extractables and Leachables Safety Information Exchange Database)
- Stabilizers, accelerators, intermediates, residual monomers, antioxidants, food packaging contaminants and printing ink components and their breakdown products

## 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 Services (optional):

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

### Method and Application Services (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 extractables and leachables faster. Visit [www.agilent.com/chem/extractables-leachables](http://www.agilent.com/chem/extractables-leachables)



## Complete your E&L 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 1260 or 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 extractables and leachables 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:

### Extractables and Leachables PCDL (G6890CA)

#### Required but not included with the E&L PCDL:

Agilent 1260 or 1290 Infinity II LC (Ultra Clean Option)

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: Agilent Mass Profiler Software (B.07.00 or higher)

OPTIONAL: Agilent Mass Profiler Professional Software (14.5 or higher, ships with Molecular Structure Correlator B.07.00 and MassHunter Profinder B.06.00)

OPTIONAL: G6890CA #001 Installation and Familiarization Service

OPTIONAL: Method and Application Services H2149A (Americas); R1736A (other regions)

## Put your lab on the productivity fast track

Contact your local Agilent Representative or Agilent Authorized Distributor at [www.agilent.com/chem/contactus](http://www.agilent.com/chem/contactus)

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

For a description of available LC/MS Databases and Libraries, and GC/MS Analyzers, visit [www.agilent.com/chem/ms](http://www.agilent.com/chem/ms)

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