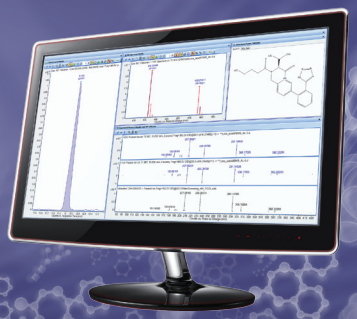
SIMPLIFY YOUR COMPREHENSIVE SCREENING OF FORENSIC TOXICOLOGY COMPOUNDS



Agilent Forensic Toxicology LC/MS Personal Compound Database and Library

Confidently perform target and suspect screening using accurate mass

Forensic toxicological analysis of biological samples is challenging due to the large number of trace-level analytes to be identified and confirmed. Staying on top of the identity of continuously evolving designer drugs is particularly difficult.

You can screen for more than 9,200 analytes by combining TOF or Q-TOF LC/MS instruments with the Agilent Forensic Toxicology Personal Compound Database and Library (PCDL), resulting in highly confident identification by accurate mass MS/MS spectra comparison. Among other compound classes, the PCDL includes over 750 designer drugs.

One outstanding feature of full spectrum analysis is the capability for retrospective analysis. 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 – which allows you to stay up to date with drugs as they hit the street.

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

- Curated accurate-mass database with more than 9,200 compounds
- Searchable user notes containing compound class tags
- Accurate-mass MS/MS spectra for more than 3,900 compounds, acquired at 3 different collision energies, plus adduct and loss spectra (over 13,500 spectra total)
- Quick-start guide with data examples and familiarization exercises
- Method setup guide that shows you how to set up acquisition methods
- Application note with detailed LC/MS method information
- Latest version of PCDL Manager Software
- Free database and library upgrades for 3 years

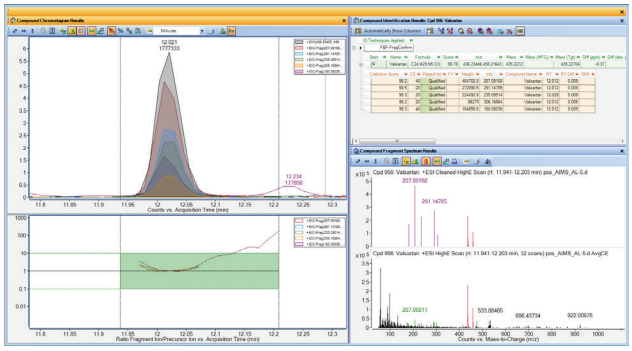
Agilent Technologies

Target and suspect screening workflows with the PCDL

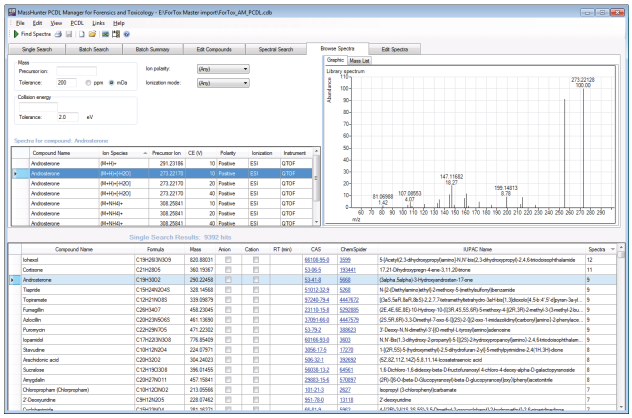
The Agilent Forensic Toxicology PCDL, combined with the accurate mass capabilities of LC/TOF and Q-TOF instruments, enables you to:

- 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
- Create a custom PCDL for a more focused screening approach
- Propose a suspect list with MS data and the "Find by Formula" algorithm
- 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

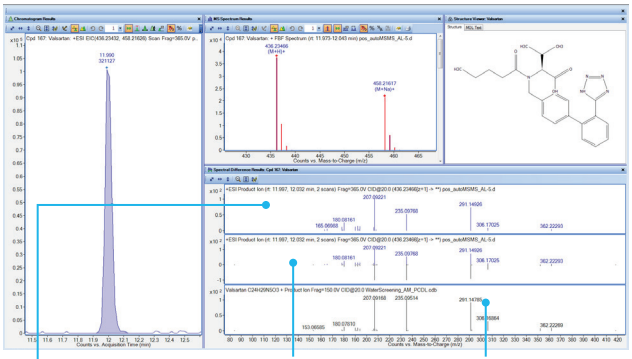
The Forensic Toxicology PCDL makes compound confirmation and data mining easier – even for high-throughput labs – to perform truly comprehensive screening of an unlimited number of compounds.



Easy data mining and unambiguous identification using All Ions Software.



PCDL Manager Software provides easy management of the database and library.



Top: Auto MS/MS spectrum

Middle: Mirror spectrum

Bottom: Library spectrum

Attain compound confirmation by library matching using Auto MS/MS.

High-sensitivity screening for forensic toxicology compounds

The Agilent Forensic Toxicology PCDL can help you to stay on top of the ever growing list of new drugs. It includes over 9,200 compounds–including the following:

Available class tags:

Human doping drugs, Designer drugs, Veterinary Drugs, Equine drugs, Pesticides, Mycotoxins, Cannabinoids, Hallucinogens, Stimulants, Benzodiazepines, Hypnotics, Neuroleptics, Barbiturates, Antidepressants, Cardiovascular Medicals, Antiepileptics, Opioids, Anabolic agents, PPCPs, Hormones, Internal Standards.

Database and library curation assure highest data quality

- 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)
- Each precursor and product ion peak corrected to theoretical accurate mass
- Spectra acquired at 10, 20, and 40 V collision energy
- Spectra measured in positive and/or negative ion mode where applicable
- Includes adduct and loss spectra
- Spectra filtered for signal intensity and curated for spectrum noise, chemical impurities, and incorrectly set instrument parameters

Application consulting tailored to your needs

Installation and familiarization:

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

Advanced application consulting:

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

Complete your 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 to suit your application.
- **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.
- **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 and unknown compounds. What's more, the Agilent Jet Stream electrospray ion source dramatically lowers detection limits.
- **Agilent LC columns, supplies, and sample prep products** increase your uptime and achieve the best scientific outcomes.

Ordering information

Forensic Toxicology Personal Compound Database and Library (G3876CA)

The following are required but not included with the Forensic Toxicology PCDL:

- Agilent 1260 or 1290 Infinity II Series LC
- 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
- OPTIONAL: G3876CA #001 Installation and Familiarization Service
- OPTIONAL: Advanced Application Consulting H2149A (Americas); R1736A (other regions)

To learn more about the Agilent Forensic Toxicology PCDL, visit
www.agilent.com/chem/pcdl

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 LC/MS Databases and
Libraries and GC/MS Analyzers

For Forensic Use.

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