STREAMLINE TARGETED SCREENING OF FORENSIC TOXICOLOGY COMPOUNDS

Agilent Forensic Toxicology tMRM Database

Minimize the need for tedious method development with a database of MRM transitions

Analyzing forensic toxicology compounds is challenging for two reasons – low concentrations and a large number of analytes to be monitored and quantified. With these variables to consider, it can be difficult to find a solid starting point for method development.

The Agilent Forensic Toxicology tMRM Database combined with Agilent Triple Quadrupole LC/MS enables you to instantly build methods for targeted screening and confident quantitation for hundreds of analytes in a single run. Much of the development work has already been completed by Agilent, leaving you more time to create quality data that can stand up to the scrutiny required in forensic toxicology investigations.

The Agilent tMRM databases contain hundreds of transition parameters for triple quadrupole LC/MS, allowing you to create MRM, dynamic MRM (dMRM), or triggered MRM (tMRM) methods. Chose the mode best suited to your analysis needs.

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

- Curated database with more than 2,800 compounds
- Up to 10 MRM transitions, fragmentor voltages and collision energies for all compounds, applicable across all Triple Quadrupole LC/MS platforms
- Quick-start guide with data examples and familiarization exercises
- Method setup guide that shows you how to create MRM, dynamic MRM, and triggered MRM methods
- Free database upgrades for 3 years

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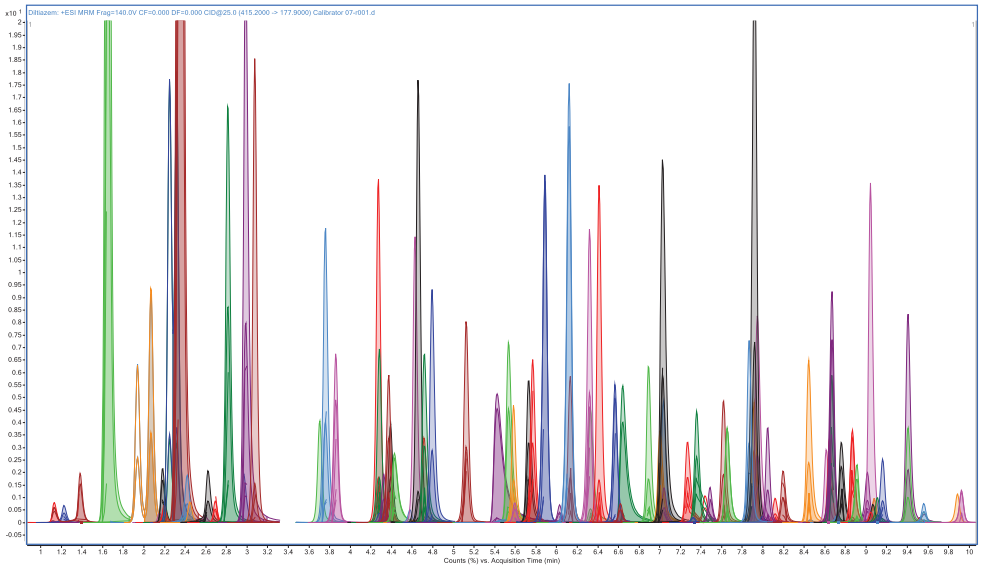
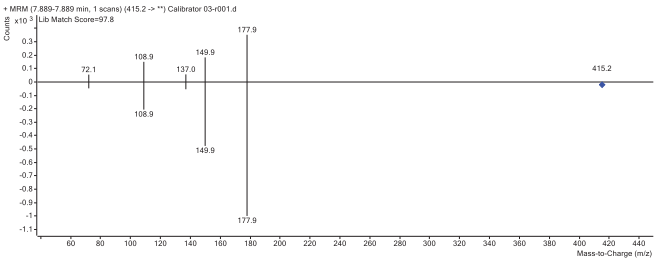
Target screening workflows with the tMRM Database

The Agilent Forensic Toxicology tMRM Database and Reference Library, combined with the high sensitivity and accurate quantitative capabilities of the triple quadrupole LC/MS system, enables different workflows, including:

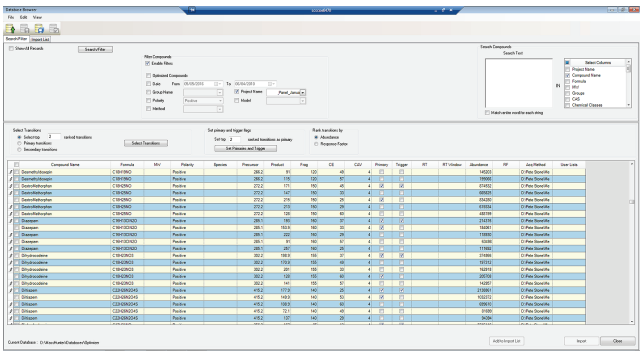
- Easily create an MRM method by importing all settings like compound names, primary MRM transitions, fragmentor voltages, and collision energies from the database. An MRM method is appropriate for fast screening and quantitation of a limited number of compounds without the need to know retention times.
- Evaluate retention times and retention time windows to update the MRM method to a dynamic MRM method. Dynamic MRM maximizes dwell time for analytes within their time window for best sensitivity. Dynamic MRM is appropriate for screening and quantitation of hundreds of analytes within one run.
- If even more specificity is needed, secondary transitions can be added to a dMRM method to create a tMRM method. Triggered MRM is particularly beneficial for isobaric compounds and compounds affected by matrix interference. Triggered MRM is compatible with the need for fast cycle times so it can be applied either to a subset of problematic compounds or to all compounds in a multi residue screen.
- Create a reference library from your data, specific to your analysis, and confirm results with a library match to confidently assess borderline results.



10-minute MRM chromatogram of 100 toxicological analytes (plus internal standards) with up to five triggered MRM transitions overlaid.



Reference library match and score for Diltiazem.



Agilent's Forensic Toxicology tMRM database ensures fast, customized method development.

Curation of the database and reference library assure highest confidence results

- Compound common name
- CAS number of the native compound
- Molecular formula
- Unit mass of neutral molecule
- MRM transitions (precursor and product m/z)
- Fragmentor voltage
- Collision energy
- Added retention times and retention time windows
- Added trigger parameters
- MRM transitions fully optimized using the Agilent MassHunter Optimizer software for more than 743 compounds
- Optimized MRM data are reviewed for correctness

Compound classes include:

Designer drugs, Cannabinoids, Hallucinogens, Stimulants, Benzodiazepines, Hypnotics, Neuroleptics, Barbiturates, Antidepressants, Cardiovascular Medicals, Antiepileptics, Opioids.

Application consulting tailored to your needs

Installation and familiarization:

- Experienced service personnel will install the tMRM database and reference library, verify all functionality 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 tMRM database by setting up targeted screening methods for your samples of interest and ensure you achieve your scientific outcome.

Complete targeted analysis workflow with leading-edge solutions from Agilent

- **MassHunter data acquisition and analysis software**
  Together with the fully integrated tMRM database, this powerful software lets you quickly generate acquisition and analysis methods, which can be modified easily to meet your needs. In MassHunter Quantitative Analysis Software, you can use batch processing to flag outliers, and view compounds at a glance to review by exception.
- **Agilent 1290 Infinity II LC and Agilent 6400 Series Triple Quadrupole LC/MS systems**
  Proven choices for quantitative applications give you unmatched separation performance, superior sensitivity, renowned reliability, and overall robustness. 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

Forensic Toxicology tMRM Database and Reference Library (G1734CA)

The following are required but not included with the Forensic Toxicology tMRM Database and Reference Library:

- Agilent 1260 or 1290 Infinity II Series LC
- Agilent 6400 Series Triple Quadrupole LC/MS System
- Agilent MassHunter Acquisition Software B.06 or higher and Windows 7 64-Bit
- Agilent MassHunter Qualitative Analysis Software B.06 or higher
- Agilent MassHunter Quantitative Analysis Software B.05.02 or higher
- OPTIONAL: G1734CA #001 Installation and Familiarization Service
- OPTIONAL: Advanced Application Consulting H2149A (Americas); R1736A (other regions)

To learn more about the Agilent Forensics Toxicology tMRM Database and Reference Library, visit **www.agilent.com/chem/tmrm**

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

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