

APPLICATION SOLUTION

FORENSIC TOXICOLOGY SCREENING

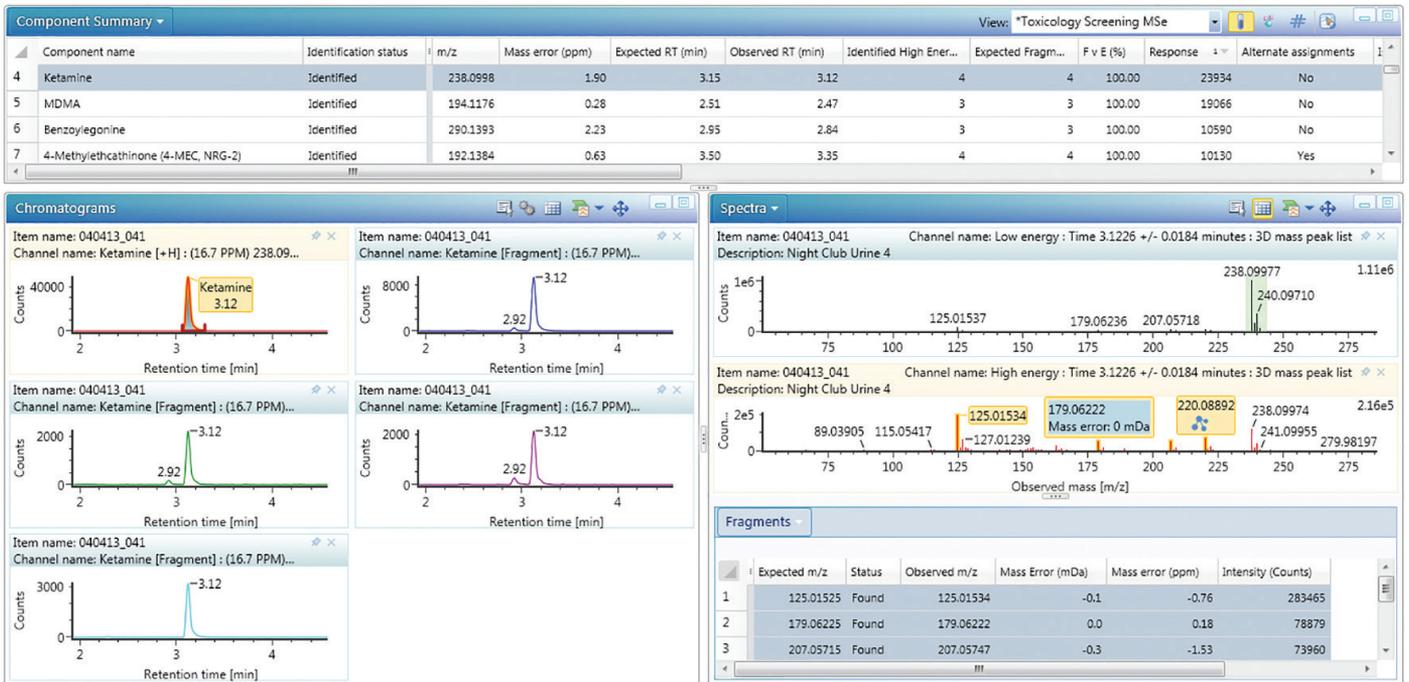


Waters

THE SCIENCE OF WHAT'S POSSIBLE.®

UNMATCHED ACCURACY AND
SENSITIVITY AT YOUR BENCHTOP.





The Toxicology Workflow Summary allows the user to review a component summary of all compounds identified in the sample through a comprehensive data summary table. In this example, Ketamine is easily identified and confirmed with the component summary and time-aligned fragment ions and high and low energy spectra summaries found in the bottom left and right sections respectively.

The most innovative screening solution ever built for forensic toxicology testing.

Forensic toxicology labs are frequently required to perform broad screening techniques on complex biological samples to identify drugs of abuse and other toxicants. The utilization of different sample matrices in routine testing combined with the variety, number and concentration of potential compounds of interest in a sample can present a considerable challenge.

Furthermore, the continuous growth of new emerging and “designer” drugs only adds to testing complexity. Ideally suited to address these analytical challenges, Waters UNIFI Forensic Toxicology screening application solution offers a number of unparalleled benefits, empowering toxicologists to streamline workflow and improve confidence in data accuracy for even the most challenging cases.

Results you can rely on with even the most challenging samples.

The Forensic Toxicology Screening Application Solution with UNIFI delivers the sensitivity, reproducibility, and ease-of-use necessary to perform broad screening techniques on complex biological samples to identify drugs of abuse and other toxicants of interest. Now, for the first time, you will be able to reliably report the presence or absence of toxicological compounds of interest, easily streamline workflows, and increase the speed of analysis for complex matrices using the scientific library functionality and flexible reporting templates.



Workflow – customized to maximize usability

- Pre-defined, toxicology workflow improves speed and ease of data review
- Data filters automatically screen data
- Workflows can be personalized and saved depending on user and application
- Allows users to quickly focus on samples that may require additional interpretation

Comprehensive exact mass toxicology library

- Combination of parent, fragment, and retention time data improves accuracy and reduces false positives
- Increased confidence in compound identification
- Enables significant time savings for users
- Includes emerging designer and synthetic drugs
- Characterization and addition of previously “unknown” compounds to the library is simple and intuitive

Fragment ion analysis – MS^E

- Improves data confidence
- Requires no method development
- Provides “snapshot-in-time” to gather all data in one run, no need for sample reinjection
- Enables retrospective analysis of unknowns

3D componentization – improved peak detection

- Better peak detection
- Reduces false positives
- Lower level peaks detected with confidence
- Cleaner, improved spectral quality

Workgroup – data security and traceability

- Best-in-class data security and traceability
- Audit trail of data processing
- Eliminates the need to generate or transfer multiple copies of data
- Saves time and reduces storage requirements
- Latest methods, libraries, data templates accessible to all

OPTIMIZED FORENSIC TESTING REQUIREMENTS.

A purpose-built collection of the best-in-class components for toxicology testing.

UNIFI is the first and only Scientific Information System that allows your laboratory to operate at the forefront of science. For the first time, you can employ consolidated state-of-the-art data acquisition, data processing, and data management requirements with access to an extensive scientific library – allowing you to combine all the components necessary for effective toxicology screening.

Unparalleled collaboration

UNIFI unleashes the power of true dynamic collaboration – changing and accelerating scientific developments and innovations. Store, make use of, and share all your data, all methods, and reports.

Make use of your prior work, as well as your colleagues' data and findings, to drive your science forward.

Science driven by collective intelligence

With UNIFI, you can always answer questions like, “What is this compound? Have I seen this before? Has anyone seen this before?”

UNIFI ensures that your lab is always starting ahead – armed with, and benefitting from, the collective intelligence of all your scientists.

And because you can immediately see what's been done in the past, you can make decisions more quickly, easily, and confidently.

The result

You can make the correct decision the first time, every time.

ACQUITY UPLC® I-Class >
Xevo® G2-S QTof
UNIFI
Methods
Toxicology
Chemistries
Toxicology Scientific Library



UNIFI SCIENTIFIC INFORMATION SYSTEM, FIRST OF ITS KIND – UNIQUELY WATERS

- Reliably detect, quantify, and report the presence of drugs and other compounds of interest, minimizing both false positive and false negative results
- Identify known and unknown compounds with the UNIFI Scientific Library
- Build a historical record of sample analysis data for retrospective review as new challenges emerge
- A next-generation solution built upon proven, category-leading Waters technology

The UNIFI advantage.

Laboratories today are being asked to work smarter, work faster, and make the most of existing resources.

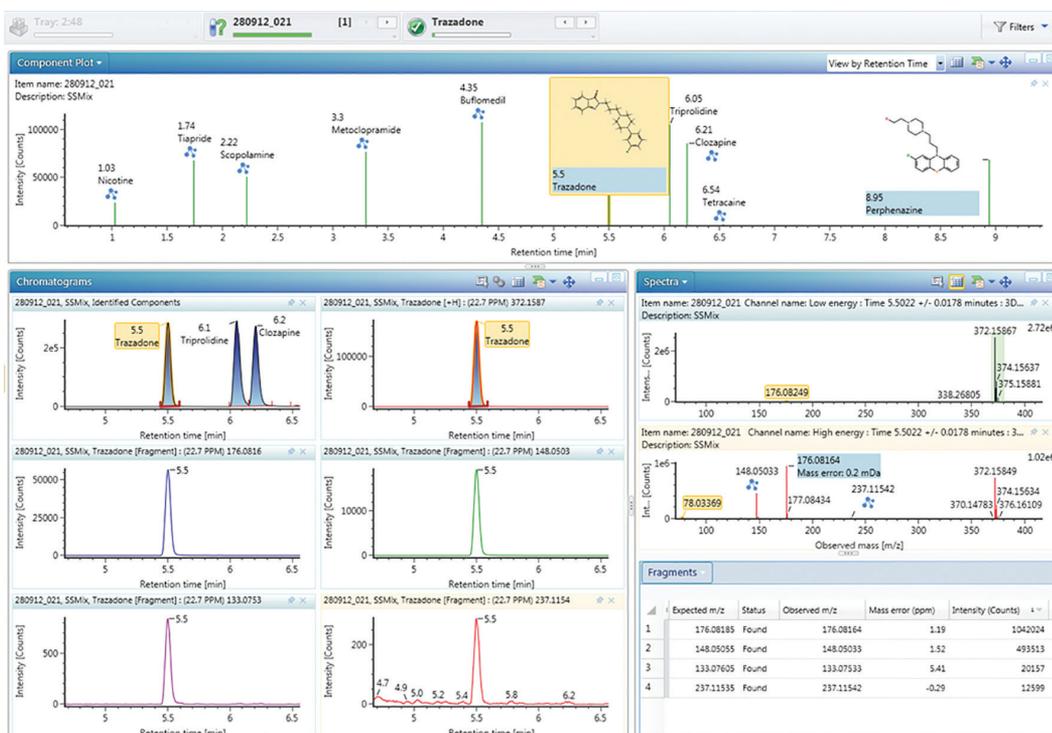
That is why the answer is UNIFI: Capture complex high-end mass spectrometry and chromatography data on one platform. Get more information from a single injection. Gain the ability to test, quantify, and confirm the presence of compounds in a single measurement.

And the result?

Save time and effort, eliminate reworking of processes, and reduce the list of compounds you have to check in during follow-up testing.

The obvious way for laboratories to meet all these demands is to be able to identify expected, as well as unexpected, drugs of abuse and other compounds in a sample – allowing scientists to see those that are of immediate concern and interest, and beyond.

This is where the UNIFI Scientific Library becomes an invaluable asset – effectively functioning as an expanding repository for scientific knowledge, constantly improving the efficacy of future analyses, and building a historical record of analyses. This allows for retrospective interrogation of data, enhancing the value of the surveillance system and reducing the fear of the unknown.



This alternative Workflow Summary shows all the components identified across the entire sample chromatogram. By highlighting a select compound, the chemical structure is shown automatically as evidenced by Trazadone at 5.5 minutes retention time.

The information rich MS^E data enables a complete data set of low and high energy spectra, enabling Toxicologists to minimize false positives and easily make identifications and confirmations in one screen.

Not just an application solution –
a total solution.

The sensitivity, specificity, mass accuracy, and resolution that can be achieved with the Waters ACQUITY UPLC I-Class System coupled to Xevo G2-S QToF make this LC-MS/MS application solution ideal for toxicological screening.

Exploiting the capabilities of the QToF instrument and the sophisticated compound elucidation software tools in UNIFI, it is possible to identify both expected and unexpected drugs of abuse and other toxicants that may be present in a sample.

All of the assigned compounds can be entered and stored in the UNIFI scientific database, enabling subsequent identifications through retrospective analysis based on ToF screening.

ACQUITY UPLC I-CLASS SYSTEM

Superior chromatographic resolving power affords the separation necessary for rapid, accurate retention time information for a very large numbers of analytes.



XEVO G2-S QTOF

Provides the ability to obtain both accurate mass precursor and fragment ions from a single injection. This allows more information to be generated on sample components, improving confidence and helping reduce false positive results.



TOXICOLOGY SPECIFIC METHOD

Ideally suited for targeted and non-targeted screening to help you derive optimal performance and accurate results from the start.



RELIABLE RESULTS FOR EVEN THE MOST CHALLENGING SAMPLES.

SALES OFFICES:

Austria 43 1 877 18 07

Australia 61 2 9933 1777

Belgium and Luxembourg 32 2 726 1000

Brazil 55 11 4134 3788

Canada 1 800 252 4752

China 86 21 6156 2666

Czech Republic 420 2 617 11384

Denmark 45 46 59 8080

Finland 358 9 5659 6288

France 33 1 30 48 72 00

Germany 49 6196 400 600

Hong Kong 852 2964 1800

Hungary 36 1 350 5086

India 91 80 2837 1900

Ireland 353 1 448 1500

Israel 9723 3731391

Italy 39 02 265 0983

Japan 81 3 3471 7191

Korea 82 2 6300 4800

Mexico 52 55 52 00 1860

The Netherlands 31 76 508 7200

Norway 47 6 384 6050

Poland 48 22 101 5900

Portugal 351 21 893 61 77

Puerto Rico 1 787 747 8445

Russia/CIS 7 495 727 4490 / 290 9737

Singapore 65 6593 7100

Spain 34 93 600 9300

Sweden 46 8 555 115 00

Switzerland 41 56 676 7000

Taiwan 886 2 2501 9928

UK 44 208 238 6100

US 1 800 252 4752

Waters Corporation

34 Maple Street

Milford, MA 01757 U.S.A.

T: 508 478 2000

F: 508 872 1990

www.waters.com

www.waters.com/forensics

Waters

THE SCIENCE OF WHAT'S POSSIBLE.®

Waters, The Science of What's Possible, ACQUITY UPLC, UNIFI, and Xevo are registered trademarks of Waters Corporation. All other trademarks are the property of their respective owners.

©2013 Waters Corporation. Printed in the U.S.A.
December 2013 720004830EN LM-KP