


LC-MS/MS for Forensic Screening



SIECI Triple Quad™

System

- Quantitation
- ID with NMRM ratio


SIECI QTRAP® system

- Quantitation
- ID with NMRM ratio
- **ID with MS/MS library searching**

GTOF MS

- Quantitation
- ID with accurate mass
- ID with MS/MS library searching
- **ID True unknowns**
- **Retrospective data processing**

Increased Confidence in compound ID

 **SIECI**
The Mass of Choice

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With the sharp rise in the number of novel psychoactive substances (NPS) entering the market, forensics laboratories must have the best tools available to analyze them. LC-MS/MS is a highly sensitive and specific approach, that enables forensic toxicology laboratories to detect and identify, therapeutics and illicit drugs, as well as their metabolites.

- Challenges for NPS screening
- LC/MS workflows for rapid identification and quantification of NPS
- How SCIEX OS Software for NPS detection is streamlining data processing

Novel psychoactive substances (NPS) pose significant risks to public health and safety, therefore timely and comprehensive drug screening approaches are vital in the forensic laboratory. Building on the ability of liquid chromatography (LC) combined with tandem mass spectrometry detection (LC-MS/MS, LC-QTOF-MS) to accurately identify novel drugs in complex matrices, SCIEX have developed a comprehensive drug screening workflow for the analysis of NPS from whole human blood samples.

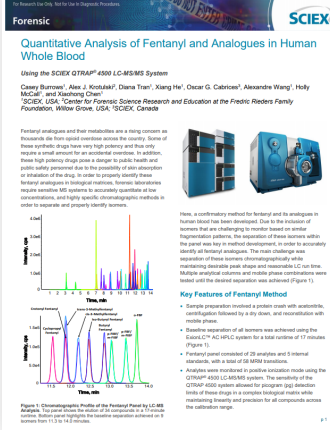
- The key features of SWATH Acquisition for NPS identification and quantification
- How SWATH Acquisition is combined with SCIEX OS Software to create a comprehensive NPS screening workflow

One of the challenges associated with NPS analysis is the range of concentrations observed. If the concentration of NPS analytes fall outside of the calibration range, the sample will need to be diluted so that accurate measurements can be made.

The SCIEX Triple Quad™ 5500+ LC-MS/MS System – QTRAP® Ready is a highly selective and sensitive method with a wide linear dynamic range. It enables quantitation across a wide concentration range, reducing unnecessary sample preparation and re-analysis.

- The key features of this method for forensic studies
- The benefits of combining it with the High Energy Dynode (HED) detection system

Technical note



Quantitative analysis of fentanyl and analogues in human whole blood

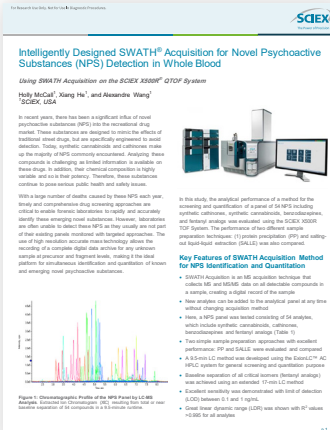
The potency of fentanyl analogues and their metabolites mean that only a small amount is required to cause an accidental overdose. As the opioid crisis continues to pose a significant threat, it is therefore vital that forensic laboratories can accurately identify these substances in biological matrices.

To achieve this, mass spectrometry (MS) systems and highly specific chromatographic methods are required to quantitate these opioids at low concentrations and separate isomers before identification, respectively.

From this technical note you will discover:

- The key features of the fentanyl method
- Why combining the QTRAP® 4500 LC-MS/MS System and the ExionLC™ AC System are beneficial for fentanyl analysis

Technical note



Intelligently designed SWATH® Acquisition for novel psychoactive substances (nps) detection in whole blood

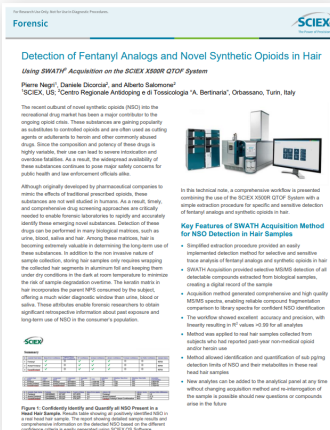
Novel psychoactive substances (NPS) have different chemical compositions and potencies compared to traditional street drugs. This makes detection and analysis challenging. High-resolution accurate mass spectrometry (HRMS) creates a complete digital data archive for unknown samples at precursor and fragment levels, making it an ideal platform for simultaneous identification and quantitation of known and emerging NPS.

SWATH Acquisition is an MS acquisition technique that collects MS and MS/MS data on all detectable compounds in a sample.

From this technical note you will learn more about:

- The key features of SWATH Acquisition for NPS identification and quantitation
- A study evaluating the analytical performance of the SCIEX X500R QTOF System for NPS screening

Technical note



Detection of fentanyl analogs and novel synthetic opioids in hair

The variability in the composition and potency of novel synthetic opioids (NSO) compared to traditional opioids can result in severe intoxication and overdose fatalities. NSO are detected in many different biological matrices, however, hair is a particularly valuable sample used to detect long-term use.

The development of comprehensive screening methods will provide law enforcement agencies and health professionals with a clearer picture of long-term use drug use, their evolution in the consumer market and consumption trends in the specific populations.

From this technical note you will discover:

- The features of the SCIEX X500R QTOF System
- The benefits of combining it with a simple extraction procedure

Technical note

Streamlined Unknown Screening for Postmortem Analysis
 Using the SCIEX X500R QTOF System and SWATH® Acquisition in a Forensic Toxicology Laboratory
 Pierre Nègy, Oscar G. Cabranes, Dean Finch, Melanie Stauffer, Nadine Koenig, Derrick Shulerberger, Jennifer Ginnell and Adam M. Taylor
 SCIEX USA, Yeast Health Laboratories, USA, SCIEX Canada

Gathering evidence to determine the cause of death in postmortem is the domain of the police, coroner and the judicial process. To this end, accurate identification of drugs present in postmortem samples is critical for forensic toxicologists to successfully conduct case examinations as the findings of these examinations often have important legal and public safety implications around cause of death and other related anatomical events.

The rapid emergence of novel psychoactive substances (NPS), designer drugs and the abuse of prescription drugs have led to a need for more robust and comprehensive drug screening approaches. Traditionally, screening of drug samples are often performed by immunoassay or GC-MS. Immunoassay techniques are often not sensitive enough for these compounds and lack selectivity. GC-MS requires sample derivatization and lengthy chromatographic runs to accurately identify NPS and other drugs present in a biological postmortem sample. As a result, there is a need for rapid and robust screening methods that allow accurate identification of NPS and other drugs with a high level of sensitivity and selectivity.

High-resolution mass spectrometry (HRMS) in the forensic laboratory allows toxicologists to rapidly obtain complete chemical profiles from biological samples. The acquisition of accurate mass, analysis specific MS/MS spectra often provides increased confidence in compound identification in low sample concentrations.

In the forensic note, a comprehensive drug screening workflow for the analysis of postmortem blood samples is described. The workflow was developed using a targeted sample preparation approach in combination with SWATH Acquisition on the SCIEX X500R QTOF System.

Key Features of Postmortem Method

- Postmortem panel consisted of 131 drugs with limits of detection (LOD) down to the sub-ng/ml range
- Sample preparation was significantly simplified, using a protein precipitation with methanol and acetonitrile, followed by microfiltration with mobile phase
- Reduced and reliable chromatographic separation was achieved using the selected² Acquisition for SWATH[®] component using the EasyLC™ AC-MS/MS system
- Analysis were monitored in positive ionization mode using SWATH Acquisition on the SCIEX X500R QTOF with SCIEX OS Software
- The method allowed identification and quantification of neoprenes (ng) detection limits of these drugs in a complex biological matrix

Figure 1. Compound library of Analyte Present in an Postmortem Blood Sample
 An example of the compound library used for the analysis of postmortem blood samples. The library contains 131 compounds, including 100 known drugs and 31 novel psychoactive substances (NPS). The library is organized by chemical class and includes the molecular weight, retention time, and MS/MS spectra for each compound.

Streamlined unknown screening for postmortem analysis

Accurate identification of drugs in postmortem samples enables forensic toxicologists to successfully determine the cause of death and it is beneficial for public interest and the judicial process. Traditional methods for post-mortem drug screening include immunoassays and gas chromatography mass spectrometry (GC-MS), however, their limitations have led to a search for more rapid and robust screening methods with higher levels of sensitivity and selectivity.

High-resolution mass spectrometry (HRMS) is a technique that can rapidly obtain complete chemical profiles from biological samples with increased confidence at low analyte concentrations.

From this technical note you will uncover:

- The key features of the postmortem method
- The benefits of SWATH Acquisition with the SCIEX X500R QTOF System for screening in postmortem analysis

Technical note

Detecting a New Wave of K2/Spice in Human Urine
 An Analytical Method for the Identification of JWH-018, JWH-073, JWH-081 and JWH-250 using the QTOF MS-ESI/MS System
 Alexander Wang, Brent Dawson, Hua-Fan Liu
 SCIEX, Redwood City, CA

Purpose
 The purpose of this document is to describe an updated version of the screening method for the active ingredients in K2/Spice blends. Previous methods have been developed for the detection of JWH-018 and JWH-073 in human urine. This new method has been expanded to include JWH-081 and JWH-250, as well as their metabolites. This screening method takes advantage of the QTOF system to provide an enhanced detection capability (DC) using multiple reaction monitoring (MRM) as a screen and an automated reporting and interpretation protocol on SCIEX OS. SCIEX OS is used to search against an internal reference library for metabolites.

Introduction
 In 2010, the Drug Enforcement Administration announced that they would be temporarily controlling five synthetic cannabinoids: JWH-018, JWH-073, JWH-081, JWH-250 and JWH-251. These compounds are synthetic cannabinoids that act as CB1 and CB2 receptor agonists. Since their introduction, they have been found in human urine samples. The major challenge for screening and has resulted in efforts to expand original screening methods so that they can detect the metabolites of every active ingredient.

Key Features of Hybrid Linear Ion Trap Technology

- Exceptional peak separation and ion trap sensitivity allow identification, characterization, confirmation, and quantification of low abundance analytes with a high degree of confidence
- Positive ionization mode for efficient identification, characterization, confirmation, and quantification – all in a single experiment
- LC/MS/MS column set provides greatly reduced dead time, allowing a trace in sensitivity, allowing much larger injections
- Broad linear dynamic range provides for high quantitative capabilities and accurate identification of analytes in complex matrices
- Positive ionization mode, including heated ion and precursor ion scans, can be used to identify compounds to enhance experimental selectivity

Figure 1. Chemical structures of JWH-018, JWH-073, JWH-081, and JWH-250
 The figure shows the chemical structures of four synthetic cannabinoids: JWH-018, JWH-073, JWH-081, and JWH-250. Each structure is labeled with its corresponding chemical name and molecular weight.

Detecting a new wave of k2/spice in human urine

In 2010, the Drug Enforcement Administration (DEA) announced that they would be temporarily controlling five synthetic cannabinoids. However, unregulated chemicals - which act as cannabinoid agonists at CB1 and CB2 receptors - have since emerged to replace these controlled substances.

Parent drug compounds are metabolized within just a few hours; therefore they may only be present at low quantities in human urine samples. This short window is a major challenge for screening and has resulted in efforts to expand original screening methods so that they can detect the metabolites of every active ingredient.

From this technical note you will learn about:

- Hybrid linear ion trap technology
- An updated version of the screening method used for the active ingredients in K2/Spice blends

Website

Designer Solutions for Designer Drug Analysis

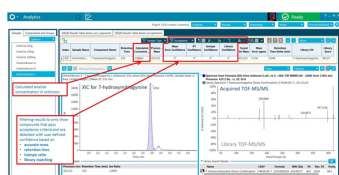
Drug testing innovations to find and ID novel and emerging psychoactive substances

SCD-0017-10-2284

For Research purposes only. Not to be used in diagnostic procedures.

Multi-target screening for standard lists of forensic drug compounds is highly useful in forensic analysis. However, with novel psychoactive substances (NPS) being developed every day, there is now the need to detect and identify assorted chemical compounds that may not be well-characterized or identified as part of a standard drug compounds list.

High resolution mass spec technology such as the X500R QTOF is a powerful tool for forensic researchers investigating their samples for unknown compounds, drug metabolites, unknown chemicals or hazards, or unknown novel psychoactive substances that have never been previously detected or characterized.



The benefits of high resolution mass spec for forensic investigations of novel psychoactive substances include:

- Sensitivity to detect very low levels of unknown chemical compounds
- SWATH[®] analysis to discover new synthetic compounds as they emerge into forensic toxicology
- Ability to leverage MS/MS fragmentation information for accurate chemical characterization
- Ability to simultaneously screen for known targeted forensic compounds in the same analysis

Designer solutions for designer drug analysis

High-resolution mass spec technology such as the X500R QTOF System is a powerful tool for forensic researchers investigating their samples for unknown compounds, drug metabolites, unknown chemicals or hazards, or unknown novel psychoactive substances that have never been previously detected or characterized.

From this resource you will discover:

- The benefits of HRMS for forensic investigations of NPS
- Links to useful resources, educational content, products and services

Technical note

Forensic

Rapid Screening of 65 Common Drugs and Drug Metabolites in Urine and Blood Using High-Resolution Mass Spectrometry

Using the SCIEX X500R QTOF System with an ExionLC™ AD System

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SCIEX, Shanghai, *Former Shanghai Public Security Department

Drug abuse has become one of the most serious social issues worldwide as drug use continues to pose a threat to social stability and economic development. As the usage of new designer drugs continues to pose public health and safety problems, drug testing remains one of the most effective measures for global drug control. As some drugs are rapidly metabolized in the body, however, the ability to swiftly detect them and their metabolites in the blood and urine of drug users is paramount for law enforcement and forensic investigations, who require sensitivity and specificity. Hence, a strategy is required that provides accurate and accurate drug intake information to the public, governmental, legal and medical sectors so that the appropriate course of action can be taken following the results of a drug test.

The SCIEX X500R QTOF System is a fast scanning, high-resolution mass spectrometer that provides accurate, reliable, accurate mass analysis for compound screening, and high-resolution accuracy requires for compound confirmation in a single analysis. The high-resolution mass spectrometer provides the rigorous, rapid, sensitivity and resolution that is essential to support field authority investigations. The X500R QTOF System is therefore ideally suited for forensic analysis of drug and drug metabolites as well as screening and confirmation in complex biological matrices.

Figure 1: High Sensitivity and Accuracy of the X500R QTOF System

The graph displays the detection of 65 common drugs and drug metabolites in urine and blood samples. The x-axis represents the retention time (min) and the y-axis represents the relative intensity. The data points are clustered into three groups: Group 1 (1-10 min), Group 2 (10-20 min), and Group 3 (20-30 min). The detection limit is 1 ng/mL for Group 1, 10 ng/mL for Group 2, and 100 ng/mL for Group 3.

Rapid screening of 65 common drugs and drug metabolites in urine and blood using high-resolution mass spectrometry

Drug abuse is one of the most serious social issues worldwide, as it continues to threaten social stability and economic development. Drug testing remains a highly effective measure of global drug control. However, the rapid metabolism of drugs in the body limits the ability to detect them and their metabolites with high sensitivity and selectivity.

The SCIEX X500R QTOF System is a fast scanning, high-resolution mass spectrometer that provides reliable and accurate drug intake information to support field authority investigations.

From this technical note you will learn more about:

- The key features and benefits of the combined acquisition method for drug and drug metabolite detection in blood and urine samples

Technical note

Forensic

Multi-panel detection of drugs and drug metabolites in hair samples using a comprehensive extraction method

Using the SCIEX QTRAP® 6500+ LC-MS/MS System

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The ability to accurately identify the presence of a variety of drugs and drug metabolites in biological specimens is a critical aspect in any forensic and clinical toxicology investigation as it provides a comprehensive picture of past drug exposure, recent consumption, a history of the neurodegenerative substances in the human body. Detection of these substances can be performed in several biological matrices including blood, urine, hair, sweat and saliva. Although urine and blood testing are the most common forms of drug testing, hair analysis has gained considerable attention over the years as a method enabling the determination of recent drug use as well as the long-term drug use through segmental analysis. Additional benefits of hair testing include the non-invasive nature of sample collection and the ease of sample storage and transportation. These advantages considerably increase the rate of sample detection and degradation over time as well as the risk of exposure to biohazards. As a result, these methods are being the superior option of hair testing to address a wide range of challenges including comprehensive analysis, QTOF screening, therapeutic drug monitoring and drug-related issues (DRI), investigations, as well as providing a broader picture of past drug consumption and abuse with a longer detection window (months to years).

Figure 1: High Sensitivity and Accuracy of the QTRAP 6500+ LC-MS/MS System

The graph displays the detection of 65 common drugs and drug metabolites in hair samples. The x-axis represents the retention time (min) and the y-axis represents the relative intensity. The data points are clustered into three groups: Group 1 (1-10 min), Group 2 (10-20 min), and Group 3 (20-30 min). The detection limit is 1 ng/mL for Group 1, 10 ng/mL for Group 2, and 100 ng/mL for Group 3.

Multi-panel detection of drugs and drug metabolites in hair samples using a comprehensive extraction method

Although urine and blood testing are the most common forms of drug testing, hair analysis has gained considerable attention over the years as a method enabling the determination of recent past drug use as well as the long term drug use through segmental analysis.

The combination of an easily implemented sample extraction procedure with the sensitivity of the SCIEX QTRAP® 6500+ LC-MS/MS System has enabled accurate identification and sensitive quantification of a wide range of chemically-diverse analytes.

From this technical note you will learn more about:

- The benefits of using this comprehensive workflow for the detection of drugs and their metabolites in hair samples

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