

thermo**scientific**

# REMOVING DOUBT IN FORENSIC SCIENCE

Mass Spectrometry Workflows  
Solving Forensic Cases

**ThermoFisher**  
SCIENTIFIC

# INTRODUCTION

While the forensic market is estimated to grow at a rate of 7% annually, the adoption of mass spectrometry-based workflows is outpacing market growth across the globe.

This is in part due to the continued rise in the manufacturing and trafficking of new designer drugs, which are easily obtained via the Internet and intentionally mislabeled as herbal incense to skirt current anti-drug laws. As many as one new designer drug is introduced to the street each week, outpacing traditional interdiction approaches.

This e-book will examine current trends and pain points in forensics and show how forensic scientists and institutions around the world are addressing these by adopting new solutions to empower quicker, more cost-effective casework results.

Because when justice is on the line, so is your reputation. And mass spectrometry-based solutions help find the truth.





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# Chapter 1

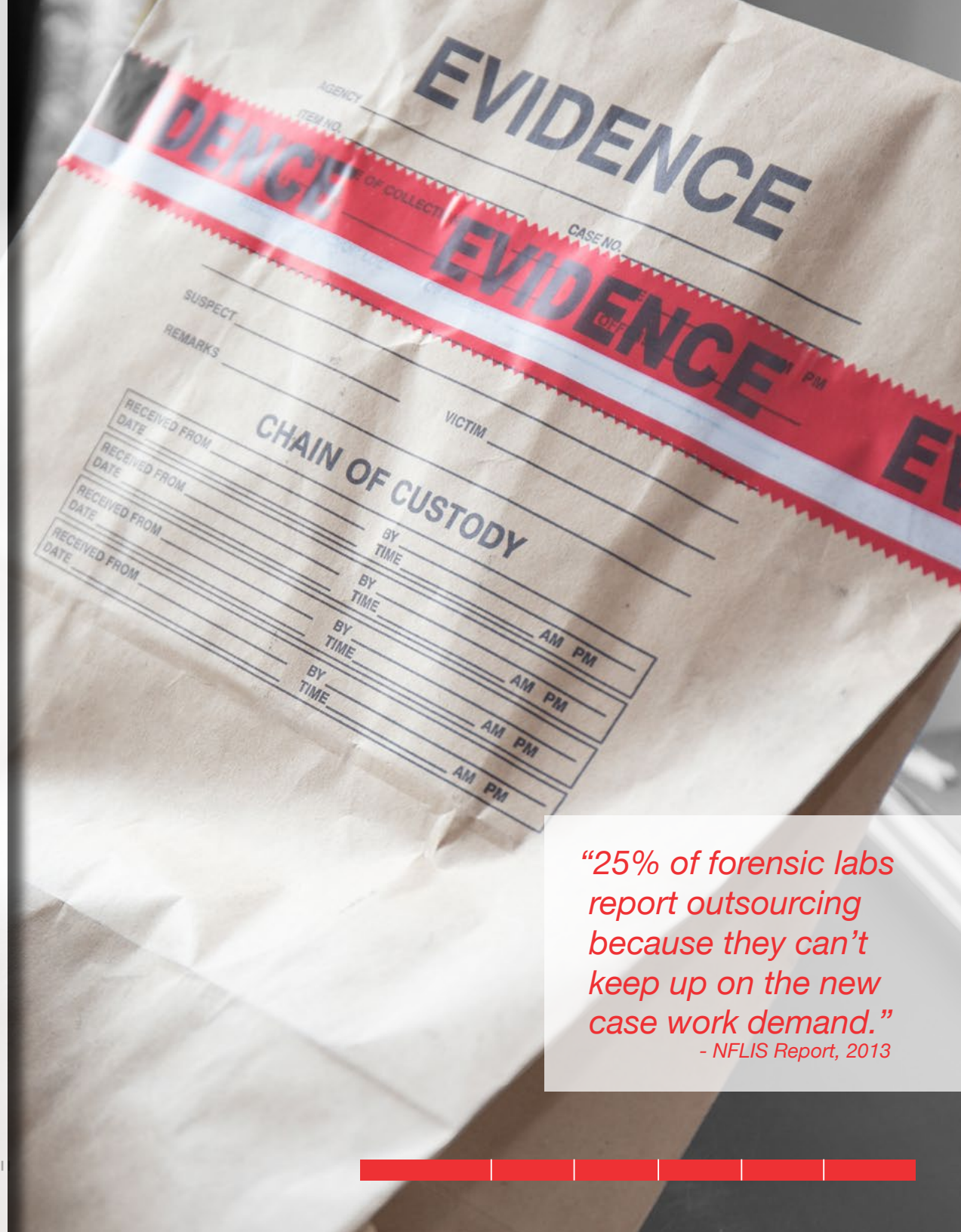
## TRENDS AND PAIN POINTS

Advances in forensic laboratory technology and the need to adopt new innovations, such as high resolution accurate mass spectrometry (HRAM), direct interfaces which eliminate complex workflow steps, and industry crowd-sourced libraries, seem like practical solutions.

However, with new technology comes the need to train or employ highly qualified forensic analysts, as well as validate new laboratory procedures. And decentralized forensic laboratory networks continue to impact state or countrywide efficiencies.

### Laboratory Caseload and Funding

Government forensic labs continue to face funding challenges. Forensic caseloads have increased as a result of more awareness of new forensic chemistry technologies and capabilities that solve more crimes, inefficient lab networks, and the slow access to new technology due to long asset acquisition justification cycles.



*“25% of forensic labs report outsourcing because they can’t keep up on the new case work demand.”*

*- NFLIS Report, 2013*

## Outdated Technological Approaches

Because funding is a challenge and training skilled forensic analysts in new techniques isn't easy, many forensic laboratories continue to maintain time-consuming methodologies – often requiring multiple orthogonal tests to close a single case. Adopting and validating new scientific techniques for forensic casework isn't easy and is often met with resistance.

## Emerging Drug Entrants

Forensic analysis laboratories continue to see a rise in first-time identified novel psychoactive substances (NPS). A recent study by the U.S. Drug Enforcement Administration's National Forensic Laboratory Information System found that, of 400 U.S. forensic laboratories surveyed, around 30% reported their drug chemistry caseloads increasing year-on-year. Almost 60% of those queried said the influx of newly identified drugs was a major contributor to their backlog.

## Regulatory Changes

Legal and regulatory changes require constant process optimization, new methods development and validation, and technology upgrades. For instance, once an illegal substance, cannabis is increasingly accepted and approved for medicinal – and in some cases, recreational use, in local jurisdictions across the globe. Law enforcement and forensic laboratories are now faced with determining new standards for “under the influence”.

## Changing Face of Crime

The economic impact of terrorism is challenging to calculate. It's difficult to even gauge direct costs like loss of life and property damage, let alone indirect effects like reduced productivity or weakened consumer sentiment. The 2015 Global Terrorism Index report estimates that terrorism costs the global economy \$52.9 billion, in addition to the \$114 billion which countries' national security agencies spent on counter-terrorism.

## Changing Case Requirements

In 2013, the NFLIS (National Forensic Laboratory Information System) reported more than 35% of forensic labs had to perform quantitative analysis to support statutory and prosecutor requests. Popular techniques can screen for a variety of compounds, but are unable to adequately quantify or determine purity ratios. Since purity is likely to increase adverse pharmacological effects, more jurisdictions want to establish the level of sanction associated with purity for prosecution purposes.

## Shifting Roles

As forensic science and technology become more complicated and difficult for the layperson to understand, scientists will become increasingly important case advocates. Laboratory technical leaders will increasingly drive key investigative decisions, moving from a supporting role to directing the efforts of investigators where empirical science and cutting-edge technology will prevail.

## What's next?

Across the globe, forensic laboratories just like yours are investigating the latest technology to advance their forensic science quickly and cost effectively while reducing the potential risks inherent with an optimized workflow.

Laboratory consolidation or centralization is at the forefront of discussion among both the National Academy of Sciences and the Netherlands Forensic Institute to improve the quality of forensic science and to achieve efficiencies currently unattainable.



# Customer Spotlight:

## LGC

Because the majority of psychoactive substances are not detectable using traditional drugs-of-abuse analysis methods, LGC needed to deploy the latest state-of-the-art mass spectrometry techniques to offer a broad coverage, sensitive, and most importantly, 'current' screening and confirmation service to detect the use of new compounds, including piperazines, cathinones, tryptamines, phenethylamines, synthetic cannabinoids, and many others.

With over 30 years' experience in drug testing and a proven track record of introducing new technology to advance laboratory capabilities with the most recent technology, Simon Hudson, Technical Director of the Laboratory and Managed Services (LMS) division of LGC, discusses the advantages of targeted and untargeted forensic drugs-of-abuse screening using High Resolution Accurate Mass (HRAM) liquid chromatography-mass spectrometry (LC-MS) with Thermo Scientific™ Orbitrap™ technology.

[Watch the video](#)



## Chapter 2

# NOVEL PSYCHOACTIVE SUBSTANCES

The recent influx of the synthetic opioid fentanyl in the U.S. represents what some are calling the 'new heroin' epidemic. Fifty times more potent than heroin, fentanyl was originally developed as a prescription painkiller for terminally ill cancer patients, and those with severely debilitating pain. In order to cut costs, some drug traffickers are now using fentanyl to lace diluted heroin. As smaller amounts can be manufactured and shipped, its potency also makes it easier to evade detection. According to The New York Times, in the U.S. fentanyl drug seizures increased from 618 in 2012 to 4,585 in 2014, an increase of over 640% in just two years<sup>1</sup>.

What's more, the illegal trade in fentanyl has evolved to stay ahead of drug detection and import/export laws. Illegal drug manufacturers are routinely modifying the chemical structure of synthetic designer drugs, making them not readily detected by traditional targeted analysis methods such as immunoassays or by conventional single or triple quadrupole mass spectrometers.

1. [http://www.nytimes.com/2016/03/26/us/heroin-fentanyl.html?\\_r=1](http://www.nytimes.com/2016/03/26/us/heroin-fentanyl.html?_r=1)

*“More than 34 tons of novel psychoactive substances seized in 2014 globally and more than 75 new substances reported to UNODC.”*

*- World Drug Report, 2016*





The emergence of new drug variants isn't just a problem in the U.S. According to figures reported by the United Nations Office on Drugs and Crime (UNODC), the number of NPS reported worldwide has grown significantly, with the largest classes being synthetic cannabinoids, stimulants and hallucinogens.

Ironically, part of the reason for the influx of new NPS is the success of forensic screening and the UNODC's Early Warning Advisory (EWA) system, which enables greater sharing of information about NPS between countries. As more regions regulate and ban substances, and advances in analysis technology make drugs easier to identify, suppliers are forced to reformulate to evade detection.

With the emergence of NPS, forensic laboratories are under increasing pressure to cast their net wider. It takes time and resources to identify new compounds, develop new screening procedures, and revalidate methods. Fortunately, advances in MS and cloud-based libraries are helping labs expand their capabilities and screen for unknown analytes more efficiently.

## Exact Mass, Full-Scan MS

Forensic laboratories are being forced to employ alternative strategies in order to detect new derivatives of NPS. Advances such as high-resolution accurate-mass (HRAM) Orbitrap technology are helping laboratories do this more reliably with the use of highly accurate mass full-scan analysis, down to 1 ppm with 5 to 6 decimal places. Exact mass detection and unmatched resolution allow forensic labs to accurately identify new untargeted drug derivatives.

## Spectral Sharing is Key

Spectral library content and the ability to share information across the Forensic community in real-time is necessary to speed up untargeted screening for new analytes. Laboratories traditionally purchase off-the-shelf content to store locally, build their own library or follow social SWGDRUG updates. However, incorporating cloud-based solutions can help forensic labs in one jurisdiction easily share information instantaneously with another jurisdiction, or even globally, in order to catch and regulate new drug variants quickly.



# Customer Spotlight:

## LIATF

Analyzing more than 7,000 biological samples annually, in a variety of sample matrices including blood, urine and hair, for forensic cases involving driving under the influence of alcohol and drugs, compliance program testing, drug-facilitated crimes, and post-mortem toxicology isn't easy.

Chain of custody is established when samples are collected, and then it is maintained during the entire analytical process. Leading forensics labs like the Laboratorio di Igiene Ambientale e Tossicologia Forense (LIATF) are increasingly relying on more advanced MS technology. For all sample types, the ability to identify drug metabolites is key to reliable detection.

In addition to traditional drugs of abuse, samples increasingly contain designer drugs and NPS for which certified reference materials and scientific data are not always available. Learn how LIATF is solving forensic challenges as they arise using the latest technological advances.

[Watch the video](#)



# Publication Spotlight:

## ORIGIN OF ANALYSIS

Stable isotope analysis can measure isotopic signatures with extreme precision to gain unique insights into the history and origin of compounds found in complex samples. Because the isotope ratios of elements become locally enriched or depleted through a variety of kinetic and thermodynamic factors, measurement of isotope ratios can be used to differentiate between samples which otherwise share identical chemical composition.

For example, determination of the geographic origin of illicit cocaine and heroin, the most widely used narcotic drugs in the Western Hemisphere, has been the focal point of intense study by the forensic community for a few decades.

Some studies have focused on identification of trace residues present in the illicit drug, or on trace alkaloids co-extracted along with the cocaine or morphine, but provided limited value. Most were only useful in determining the processing methods used in different regions. While valuable, the information has limited applicability if the plant material or extractions were transported for final processing elsewhere.

By using Isotope Ratio Mass Spectrometry (IRMS), forensic scientists are able to predict country of origin of cocaine<sup>2</sup>.

2. Geographically Sourcing Cocaine's Origin – Delineation of the Nineteen Major Coca Growing Regions in South America, Scientific Reports 6, Article number: 23520 (2016), Mallette, et al




## Chapter 3

# DRUGGED DRIVING AND THE IMPACT OF POLYDRUG USE ON IMPAIRMENT

In the 2014 National Survey on Drug Use and Health (NSDUH), 10 million people aged 12 or older reported driving under the influence of illicit drugs during the year prior to being surveyed.<sup>4</sup>

After alcohol, marijuana is the drug most often linked to drugged driving. Using validated test procedures, forensic analysts measure the level of delta-9-tetrahydrocannabinol (THC), marijuana's mind-altering ingredient, in blood samples. Since THC can be detected in body fluids for days or even weeks after use, and is often used with alcohol, it is challenging to determine the role marijuana plays in an accident. The risk associated with marijuana when used in combination with alcohol, cocaine or benzodiazepines appears to be greater than that for either drug by itself.<sup>5,6</sup>

Prescription drugs are more frequently linked to drugged driving crashes as well. A 2010 nationwide study found that about 47 percent of drivers who tested positive for drugs had used a prescription drug, 37 percent had used marijuana, and about 10 percent had used cocaine.



*“80% reduction in alcohol impaired drivers, but up to 16% of motor vehicle crashes involve drugs (legal and illegal) other than alcohol.”<sup>3</sup>*

- NHTSA, 2015

The most common prescription drugs found were pain relievers.<sup>5</sup> However, the study didn't distinguish between medically-supervised and illicit use of prescription drugs.

## Drugged Driving Dangers

The effects of each drug differ depending on how they act on the brain. For example, marijuana or alcohol can slow reaction time, impair judgment of time and distance, and decrease coordination. Cocaine or methamphetamine tends to make drivers more aggressive and reckless. Benzodiazepines, a class of sedatives, can cause dizziness and drowsiness. All of these impairments can lead to vehicle crashes.

## Roadside Testing

A good roadside test for drug levels for polydrug use does not yet exist. When using roadside measurement techniques, police don't typically request additional drug testing if the driver has already been found to have reached an illegal blood alcohol level because there is already enough evidence to arrest and prosecute.

One 2008 NHTSA study found that 18 percent of drivers killed in a crash tested positive for at least one drug.<sup>6</sup> A 2010 study showed that 11 percent of deadly crashes involved a drugged driver.<sup>5</sup>

## BAC Challenges

Modern forensic toxicology laboratories need productivity and reliability to enable continuous, often 24/7, operations and to allow the defensible and dependable quantitative determination of alcohol content in blood. Since testing results can mean innocence or guilt, the ability to resolve all doubt is key and why labs provide replicate results and why others are considering using mass spectrometry.

3. Compton RP, Berning A. Traffic Safety Facts Research Note: drugs and alcohol crash risk. Washington, DC: NHTSA; 2015
4. Center for Behavioral Health Statistics and Quality (CBHSQ). Behavioral Health Trends in the United States: Results from the 2014 National Survey on Drug Use and Health. Rockville, MD: Substance Abuse and Mental Health Services Administration; 2015. HHS Publication No. SMA 15-4927, NSDUH Series H-50.
5. Hartman RL, Huestis MA. Cannabis effects on driving skills. Clin Chem. 2013;59(3):478-492. doi:10.1373/clinchem.2012.194381.
6. Wilson FA, Stimpson JP, Pagán JA. Fatal crashes from drivers testing positive for drugs in the U.S., 1993-2010. Public Health Rep Wash DC 1974. 2014;129(4):342-350.

# Customer Spotlight:

## ST. OLAVS HOSPITAL

In Europe, the medical forensic institutes can play a much greater role than government-funded forensic science laboratories like local municipalities in the United States. Hospitals often have departments that evolve to help support forensic casework. Toward this goal, laboratory specialists are extending the deployment of their gas chromatography (GC) and GC-MS solutions.

Last year, the Department of Clinical Pharmacology at St. Olavs Hospital (Trondheim, Norway) tested almost 100,000 biological specimens (blood, urine, serum and vitreous humor) that had been submitted to the department by donor sources or local law enforcement agencies. The laboratory's expertise is used to determine if alcohol or drugs played a role in driving under the influence (DUI) or driving while intoxicated (DWI), criminal sexual conduct, and death cases.

The use of highly sensitive systems is key in determining what, and how much, is in forensic samples. For blood alcohol levels in DUI or DWI investigations it's important to measure the ethanol concentration accurately. Norway has strict drinking and driving laws with a legal limit for blood-alcohol level of 0.02%. With a rise in polydrug use, GC-MS can be used for additional determinations in drugs-of-abuse testing or intoxications.

[Learn More](#)



# Chapter 4

## EMERGING TECHNOLOGY AND GUIDANCE RESPONSES

At this juncture, advanced technology is needed to address today's and tomorrow's anticipated forensic challenges and guidance documents which describe how to use it.

### Immunoassays Versus LC-MS

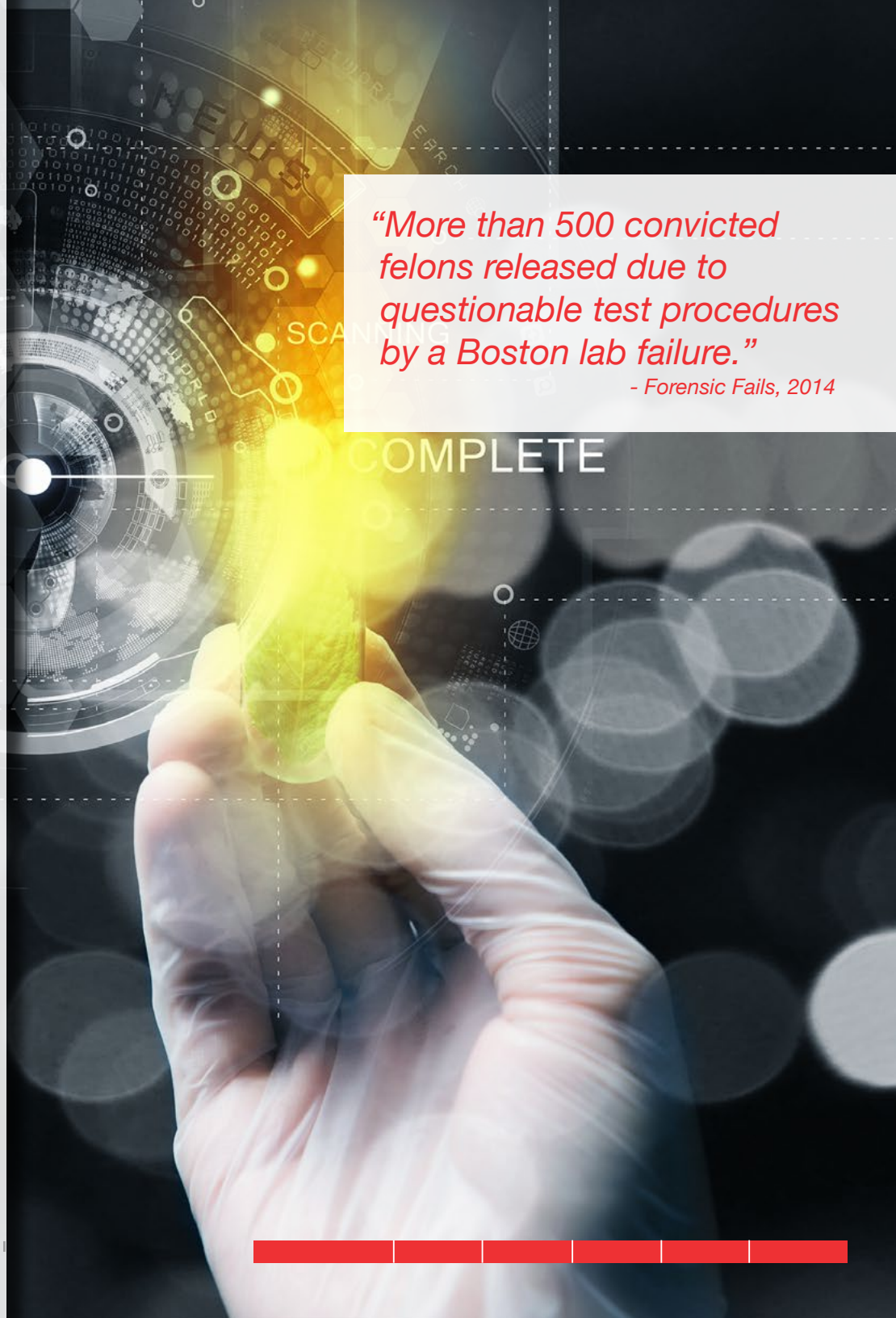
While immunoassays have been the gold standard for the past 50 years, especially in the diagnostics arena, that has not meant LC-MS isn't evaluated as an alternative to overcome some of the limitations of immunoassays.

Mass spectrometry technology is advancing, and with the limitations inherent in immunoassays, LC-MS will play a bigger role in the future. In particular, when LC-MS is used, more confidence in the accuracy of results is obtained. However, for LC-MS to have a greater role in forensics, the following need to occur:

- Easier technology adoption
- Continued performance improvements
- Guideline acceptance for use

*“More than 500 convicted felons released due to questionable test procedures by a Boston lab failure.”*

*- Forensic Fails, 2014*



## Is Forensic Science mzCloud Ready?

In the near future, local and cloud-based spectral database libraries, like mzCloud™, that contain highly curated spectral information including analyte fragmentation patterns, could be crowd sourced by fellow forensic experts. The program algorithms allow structural prediction of unknown analytes based on similarities with the fragmentation patterns of structurally related analytes. This ability to quickly recognize structural derivatives allows authorities to keep up with new threats.

The integration with MS data acquisition and software processing tools such as Thermo Scientific™ TraceFinder™ software make traditional library development and updating a thing of the past. These collaborative approaches enable drug enforcement authorities to trace points of origin and map distribution networks, which help in the fight against drug trafficking.

## In with OSAC, Out with SWG

Many agree that forensic best practices should be standardized. However, working groups like SWGDRUG and SWGTOX haven't been as effective as hoped. Meetings and funding were irregular and membership standards were inconsistent. SWG products weren't mandated or enforceable, and some were too general, with no impact studies.

The National Institute of Standards and Technology (NIST) is working with the forensic science community to establish the new Organization for Scientific Area Committees (OSAC). OSAC is part of an initiative by NIST and the Department of Justice to strengthen forensic science in the United States. The organization is a collaborative body of more than 500 forensic science practitioners and other experts who represent local, state and federal agencies, academia and industry.

OSAC is chartered with supporting the development and promulgation of forensic science consensus documentary standards and guidelines, and ensuring that a sufficient scientific basis exists for each discipline. **With the expansion of new technology, key future focus areas will be Mass Spectrometry Data Evaluation and Minimum Testing Limits for Forensic Toxicology casework.**





# Customer Spotlight:

## THE MADDY LAB

The lab replaced a panel of immunoassays (IA) with HRAM liquid chromatography-mass spectrometry (LC-MS) after a cost-recovery analysis proved the viability of the investment.

While not typical for a university-based laboratory, the Maddy Lab is entirely self-supported, and must stay revenue neutral. Running almost 70,000 samples a year, payback was within 18 months. In addition, several non-financial benefits were realized, including improved specificity (fewer false positives), improved sensitivity and surprisingly better turnaround times.

Another advantage of HRAM is the ability to re-analyze specimens. Sample data can't be re-interrogated using IA. With HRAM, the laboratory can also develop new drug detection capabilities within hours or days. If a client asks them to develop an IA test to detect a new drug, the method-development process is complex and can take up to a year. With HRAM they can complete this process within days, thus both improving client response time and tackling new substances more rapidly.

The lab now employs both Orbitrap HRAM and triple quadrupole mass spectrometers to provide the essential speed, sensitivity, stability, and accuracy required to meet the challenges they encounter in sports-doping science. These instruments provide unique "chemical fingerprints" for drug identification, making it easier for them to detect illegal doping.

[Learn More](#)



*"You need the newest equipment, highly trained staff, time and resources to develop the best anti-doping methods for detection of illegal drugs."*

*- Scott Stanley, Professor at the University of California-Davis, School of Veterinary Medicine*

# Customer Spotlight:

## LADETEC

Professor Francisco Radler, Head of the Brazilian Doping Control Lab– LADETEC–UFRJ, discusses using state-of-the-art mass spectrometry in the fight against doping. His laboratory was able to provide the highest quality results and detect the use of prohibited substances in recent global sporting events.

Aside from analyzing more than 6000 samples in a few days, Dr. Radler discusses how the lab must contend with an ever-changing game of cat and mouse between doping agencies and athletes and coaches who seek to elude detection of performance enhancing drugs.

Compared with anabolic steroids and other well-known substances, newer challenges include the use of proteins that trigger the release of growth hormones and so-called gene doping, whereby an athlete could, in theory, prompt a genetic change to enhance their performance.

[Watch the video](#)



## CONCLUSION

Adopting innovative mass spectrometry-based workflows and working with suppliers equipped to support your changing needs is key to lowering costs and obtaining results you can defend with certainty. Whether you're focused on meeting today's caseload demands or anticipating future emerging compounds of interest, we can help.

When forensic results can mean the difference between innocent or guilty, authorities depend on accurate analysis without exception. We offer laboratories reliable, cost-effective mass spectrometry-based solutions to help reveal the truth hidden in virtually any sample. Because when justice is on the line, so is your reputation.



## ADDITIONAL RESOURCES

### Sourcing cocaine with IRMS

**Authors:** Jennifer R. Mallette, John F. Casale, James Jordan, David R. Morello, Paul M. Beyer

**Publication:** Sci Rep. 2016; 6: 23520. Published online 2016 Mar 23. doi:10.1038/srep23520.

[Download](#)

### Novel psychoactive substances ID with HRMS

**Authors:** Concheiro M, Castaneto M, Kronstrand R, Huestis MA

**Publication:** J Chromatogr A. 2015 Jun 5;1397:32-42. doi: 10.1016/j.chroma.2015.04.002. Epub 2015 Apr 8.

[Download](#)

### Rapid screening for drugs of abuse in biological fluids by ultrahigh performance liquid chromatography/Orbitrap mass spectrometry

**Authors:** Jagerdeo E, Schaff JE

**Publication:** J Chromatogr B Analyt Technol Biomed Life Sci. 2016 Aug 1;1027:11-8. doi: 10.1016/j.jchromb.2016.05.010. Epub 2016 May 10.

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