

Forensic Toxicology Screening with LC-MS/MS and Automated Online Sample Preparation

Guifeng Jiang, Marta Kozak, Subodh Nimkar, Thermo Fisher Scientific, San Jose, CA, USA

Forensic Toxicology Use Only.

Key Words

- ToxSpec Analyzer
- ToxID Software
- LXQ Linear Ion Trap
- TurboFlow Technology
- Forensic Toxicology

Introduction

The quality of liquid chromatography-mass spectrometry (LC-MS) data collected in forensic drug screening applications is largely affected by sample preparation methods. Offline solid phase extraction (SPE) and liquid-liquid extraction (LLE) are the most commonly used methods. Automated online sample preparation using Thermo Scientific TurboFlow technology provides a robust front end platform for forensic drug screening, which is convenient and labor-saving.

Goal

The goal is to evaluate the performance of three sample preparation techniques – TurboFlow™ technology, SPE, and LLE – to screen 300 basic, neutral, and acidic drug compounds for forensic toxicology use.

Experimental

SPE – Mixed-mode Thermo Scientific HyperSep Verify-CX SPE cartridges (200 mg; 6 mL) were used for offline SPE. Samples of 1 mL of urine were spiked to final concentrations of 10, 100 and 1000 ng/mL with analytes of interest, as well as 100 ng/mL of three deuterated internal standards, and loaded on the SPE column. Basic, acidic, and neutral fractions were collected, combined, evaporated to dryness, reconstituted in 100 µL, and injected onto the LC column.

LLE – Toxi-Tubes® A & B (Varian) were used for offline LLE. Samples of 1 mL of urine were spiked to final concentrations of 10, 100 and 1000 ng/mL with analytes of interest, as well as 100 ng/mL of three deuterated internal standards, and then applied to the Toxi-Tube. The organic layers were transferred, evaporated to dryness, reconstituted in 100 µL, and injected onto the LC-MS.

TurboFlow Method – Urine samples were diluted in ratio 1:1 v/v with 50% MeOH containing internal standards. Fifty (50) µL of diluted sample was injected onto the TurboFlow columns. Two different chemistry TurboFlow columns were used to extract chemically diverse compounds.

A 12-minute LC method was developed for TurboFlow and LLE samples. Samples were injected onto a Thermo Scientific Hypersil GOLD PFP 100 x 30 mm, 3 µm column. A gradient method was employed with flow rates of 600 µL/min. For offline SPE samples, a 13-minute LC gradient was used with a Thermo Scientific Hypersil GOLD PFP analytical column (50 x 2.1 mm, 5 µm) and a 200 µL/min flow rate.

Mass Spectrometry

All samples were analyzed on the Thermo Scientific ToxSpec Analyzer system equipped with a Thermo Scientific LXQ

linear ion trap mass spectrometer and an electrospray ionization (ESI) source using a scan-dependent, polarity-switching method. Reports were automatically produced with Thermo Scientific ToxID automated forensic toxicology screening software, including lists of identified compounds and their matching MS/MS spectrum.

Results and Discussion

Table 1 shows limits of identification for representative compounds from the SPE, LLE, and TurboFlow methods. The lowest concentration validated was 10 ng/mL. All three methods showed comparable limits of identification. In addition, with the automated TurboFlow method, the sample quantity loaded on the column was one-quarter of that in the SPE method and one-eighth of that in the LLE method.

Table 1. Comparison of limits of identification for selected compounds

Compound	TurboFlow Method (ng/mL in urine)	SPE Method (ng/mL in urine)	LLE Method (ng/mL in urine)
Codeine	10	10	10
Hydrocodone	10	10	10
Cocaine	10	10	10
Amphetamine	10	10	1000
Stanozolol	100	100	10
Diazepam	10	10	10

Figure 1 shows the results of the identification limits of 300 drugs with the three sample preparation methods. Compared to traditional sample preparation methods, the automated TurboFlow method provides competent performance with automated online sample preparation.

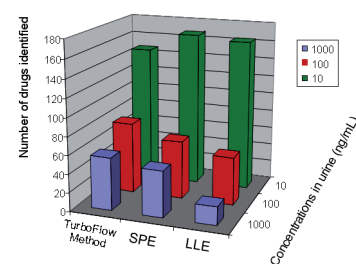


Figure 1: Limits of identification of 300 compounds

Conclusion

The TurboFlow method with the ToxSpec™ Analyzer allows for the identification of 300 drugs, with limits of detection (LODs) ranging from less than 10 ng to greater than 1000 ng per milliliter of urine. It provides an automated online sample preparation platform for forensic toxicology screening with competent performance and limits of identifications. The TurboFlow method is easier, faster, and cost efficient in comparison to traditionally used SPE and LLE methods.

In addition to these offices, Thermo Fisher Scientific maintains a network of representative organizations throughout the world.

Africa-Other
+27 11 570 1840
Australia
+61 3 9757 4300
Austria
+43 1 333 50 34 0
Belgium
+32 53 73 42 41
Canada
+1 800 530 8447
China
+86 10 8419 3588
Denmark
+45 70 23 62 60
Europe-Other
+43 1 333 50 34 0
**Finland/Norway/
Sweden**
+46 8 556 468 00
France
+33 1 60 92 48 00
Germany
+49 6103 408 1014
India
+91 22 6742 9434
Italy
+39 02 950 591
Japan
+81 45 453 9100
Latin America
+1 561 688 8700
Middle East
+43 1 333 50 34 0
Netherlands
+31 76 579 55 55
New Zealand
+64 9 980 6700
Russia/CIS
+43 1 333 50 34 0
South Africa
+27 11 570 1840
Spain
+34 914 845 965
Switzerland
+41 61 716 77 00
UK
+44 1442 233555
USA
+1 800 532 4752

www.thermoscientific.com

Legal Notices: ©2010 Thermo Fisher Scientific Inc. All rights reserved. Toxi-Tube is a registered trademark of Varian, Inc. All other trademarks are the property of Thermo Fisher Scientific Inc. and its subsidiaries. This information is presented as an example of the capabilities of Thermo Fisher Scientific Inc. products. It is not intended to encourage use of these products in any manners that might infringe the intellectual property rights of others. Specifications, terms and pricing are subject to change. Not all products are available in all countries. Please consult your local sales representative for details.



Thermo Fisher Scientific,
San Jose, CA USA is ISO Certified.

AN63131b_E 11/10S