Forensic Screening of Non-Derivatized Drugs in Urine by Comprehensive Two-Dimensional Gas Chromatography Time-of-Flight Mass Spectrometry (GCxGC-TOFMS)

John Heim

Life Science and Chemical Analysis Centre
Exploratory Research: Proof of Concept Goals

- Investigate the capability of GCxGC-TOFMS to provide practical analytical information for drug screen analysis in urine.

- Perform the study by automated sample preparation using solid phase microextraction (SPME).

- Conduct the SPME-GCxGC-TOFMS drug analysis **without sample derivatization**.

- Show calibration curve linearity for various drug classes over a concentration range from 10 to 1000ng/mL.

- Illustrate the advantages of GCxGC-TOFMS to increase peak capacity, resolution, and detectability in complex sample matrices.
GC\textsubscript{x}GC-TOFMS DESCRIPTION

[Diagram showing a GCxGC-TOFMS setup with labeled components such as Gas Chromatograph, Sampling Inlet, Carrier Gas Flow, Capillary Column, Main Oven, 2\textsuperscript{nd} dimension column, Secondary Oven, LN, Thermal Modulator, 1\textsuperscript{st} dimension column, TOFMS image.]
Experimental Methods

Sample Preparation:

• 8mL aliquots of urine were spiked with a drug mixture prepared from Sigma – Aldrich standards at concentrations from 10, 50, 250, 500, and 1000ng/mL. Hexachlorobenzene was added to each sample as an internal standard (ISTD) at 500ng/mL. Each sample was placed in a 10mL glass SPME autosampler vial and sealed.

• Samples were loaded unto an autosampler tray of the Gerstel MPS2.

• Automated SPME extraction was conducted using the Gerstel MPS2 Prepstation.
GCxGC-TOFMS with Gerstel MPS2 AUTO-SPME CAPABILITY
Solid Phase Microextraction

Syringe-type coated fiber
(50/30 μm DVB /Carboxen™/ PDMS Stable Flex)

- Direct aqueous sampling
- Headspace sampling

Advantages
- Simple
- Inexpensive
- Sensitive

Disadvantages
- Selectivity
- Limited capacity
Automated SPME Method Parameters

- **Autosampler:** Gerstel MPS2 single rail system equipped with SPME sample agitator / prepstation and SPME fiber conditioning station.
- **SPME Fiber:** 50/30 μm DVB / Carboxen™/PDMS Stable Flex
- **Agitator on Speed:** 200 rpm
- **Extraction temperature:** 37°C
- **Extraction time:** 30 minutes
- **Injection desorption time:** 2 minutes
- **Fiber conditioning station temperature:** 270°C
- **Fiber bake out (conditioning) time:** 40 minutes
Instrumental Method: GCxGC-TOFMS Analysis

Mass spectrometer: LECO Pegasus® 4D

GC: Agilent 7890 equipped with a GERSTEL MPS2 autosampler

GC Primary Column: 30m x 0.25mm id x 0.25μm film thickness, Rxi-5MS (Restek Corp.)
GC Secondary Column: 1.5m x 0.18mm id x 0.20μm film thickness, Rtx-200 (Restek Corp.)

Carrier gas: Helium @ 1.5mL / min constant flow
Injection port temperature: 260°C
Injection mode: Splitless
Transfer line temperature: 260°C

Primary column GC temperature program: Initial temperature 40°C for 2.0 min. ramped @ 6°C/min. to 290°C hold for 10.0 min.

Secondary oven GC temperature program: Initial temperature 50°C for 2.0 min. ramped @ 6°C/min. to 300°C hold for 10.0 min.

GCxGC Parameters: Modulator enabled

Modulator temperature offset: 25°C
Column offset: 10°C
Modulation period (2nd dimension separation time): 5 sec.
Hot pulse time: 0.80sec.
Cool time: 1.70sec.
The 1st dimension signal as seen by the detector.
LECO’s Dual Stage Quad Jet Thermal Modulator

Stage 1

Stage 2

COLD JETS

HOT JETS
Primary column separates components based on volatility and also generates wide bands

- The modulator focuses and re-injects time-fractions of the primary column effluent onto the second column for a second separation
  - 5+ modulations per peak

- The second column performs a rapid separation of each injected sample from the modulator based on polarity
  - $t_m \sim 1.0\ s$ for a 1.0m column
Results Discussion

- Detectability of non-derivatized drugs in the complex sample matrix urine.

- Calibration linearity over the range from 10 to 1000ng/mL

- Feasibility of this analysis for non-derivatized drugs in urine by automated SPME-GCxGC-TOFMS
TOTAL ION CHROMATOGRAM CONTOUR PLOT OF NON-DERIVATIZED DRUGS DETECTED BY AUTO-SPME-GCXGC-TOFMS

250 ng/mL drug standard spiked in 8mL aliquot of urine
The peak table above lists the minimum detection limits of 7 drugs spiked in urine at part per billion (ppb) levels.

* The relative limit of detections were calculated as an extrapolation from a ratio of concentration versus signal to noise.
Calibration linearity of greater than 90% was achieved for all components.
Extended Range Calibration for Methamphetamine

Range 1: 10 – 275 pg/μL  Linearity: R = 0.99968
## Extended Range Calibration for Methamphetamine

<table>
<thead>
<tr>
<th>Name</th>
<th>Absolute R.T. (sec, sec)</th>
<th>Range, Concentration</th>
<th>Min Valid Concentration</th>
<th>Max Valid Concentration</th>
<th>Masses</th>
<th>Quantitate Mode</th>
<th>Equation</th>
<th>Correlation Coefficients</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methamphetamine</td>
<td>1070, 1.740</td>
<td>2</td>
<td>250</td>
<td>1500</td>
<td>134</td>
<td>Equation</td>
<td>$y= +0.00116133x + 0.091255$</td>
<td>0.99483</td>
</tr>
</tbody>
</table>

**Range 2:** 250 – 1500pg/uL  
**Linearity:** $R = 0.99483$
# Calibration Table for Non-derivatized Components

Showing Linearity of > 90 % for Eight Drugs of Abuse and Metabolites.

<table>
<thead>
<tr>
<th>Name</th>
<th>Absolute R.T. (sec, sec)</th>
<th>Range, Concentration</th>
<th>Min Valid Concentration</th>
<th>Max Valid Concentration</th>
<th>Masses</th>
<th>Quantitate Mode</th>
<th>Equation</th>
<th>Correlation Coefficients</th>
<th>Curve Order</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methamphetamine</td>
<td>1070, 1.740</td>
<td>2</td>
<td>250</td>
<td>1500</td>
<td>134</td>
<td>Equation</td>
<td>$y = +0.00116113x + 0.091255$</td>
<td>0.99483</td>
<td>1</td>
<td>Analyte</td>
</tr>
<tr>
<td>Ecstasy</td>
<td>1555, 1.490</td>
<td>1</td>
<td>5</td>
<td>1500</td>
<td>135</td>
<td>Equation</td>
<td>$y = +0.00152614x - 0.0262993$</td>
<td>0.91266</td>
<td>1</td>
<td>Analyte</td>
</tr>
<tr>
<td>Hexachlorobenzene</td>
<td>1765, 1.520</td>
<td>1</td>
<td>250</td>
<td>750</td>
<td>284</td>
<td>Equation</td>
<td>NA</td>
<td>NA</td>
<td>1</td>
<td>ISTD</td>
</tr>
<tr>
<td>Cocaine</td>
<td>2285, 1.805</td>
<td>2</td>
<td>250</td>
<td>1500</td>
<td>303</td>
<td>Equation</td>
<td>$y = +0.00758373x + 0.0476363$</td>
<td>0.90428</td>
<td>1</td>
<td>Analyte</td>
</tr>
<tr>
<td>Codeine</td>
<td>2445, 1.769</td>
<td>1</td>
<td>5</td>
<td>1500</td>
<td>162</td>
<td>Equation</td>
<td>$y = +0.00070216x + 0.00415785$</td>
<td>0.95206</td>
<td>1</td>
<td>Analyte</td>
</tr>
<tr>
<td>Hydrocodone</td>
<td>2500, 1.990</td>
<td>1</td>
<td>5</td>
<td>1500</td>
<td>242</td>
<td>Equation</td>
<td>$y = +0.000750274x - 0.00944874$</td>
<td>0.96399</td>
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</tr>
<tr>
<td>6-Monoacetylmorphine</td>
<td>2555, 1.855</td>
<td>1</td>
<td>5</td>
<td>1500</td>
<td>268</td>
<td>Equation</td>
<td>$y = +0.000357057x - 0.0028296$</td>
<td>0.94953</td>
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<td>Analyte</td>
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<tr>
<td>Oxycodone</td>
<td>2560, 2.140</td>
<td>1</td>
<td>5</td>
<td>1500</td>
<td>315</td>
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<td>$y = +0.00169896x - 0.0195396$</td>
<td>0.98705</td>
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<td>Analyte</td>
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<tr>
<td>Diacetylmorphine</td>
<td>2640, 2.015</td>
<td>1</td>
<td>5</td>
<td>1500</td>
<td>327</td>
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<td>$y = +0.000761467x - 0.00359578$</td>
<td>0.97971</td>
<td>1</td>
<td>Analyte</td>
</tr>
</tbody>
</table>
The 3-dimensional surface plot of the 250ng/mL standard above was data processed at a S/N ratio of 50. Over 9000 peaks were detected.
Example of True Signal Deconvolution™ Possible by Time – of – Flight Mass Spectrometry

<table>
<thead>
<tr>
<th>Peak #</th>
<th>Name</th>
<th>R.T. (s)</th>
<th>UniqueMass</th>
<th>Similarity</th>
</tr>
</thead>
<tbody>
<tr>
<td>7277</td>
<td>Cyclohexaneacetic acid, 4-ethyl-</td>
<td>2500, 1.950</td>
<td>88</td>
<td>511</td>
</tr>
<tr>
<td>7278</td>
<td>Undeca-2,4,6,8,10-pentaenal, 11-(2-furyl)-, oxime</td>
<td>2500, 1.975</td>
<td>130</td>
<td>622</td>
</tr>
<tr>
<td>7279</td>
<td>Hydrocodone</td>
<td>2500, 1.990</td>
<td>242</td>
<td>893</td>
</tr>
</tbody>
</table>
A) above shows the deconvoluted mass spectra for peak 7279. B) above shows the library match for Hydrocodone with a match similarity of 893.
3D Plot of 20ng/mL TMS-derivatized Steroids in urine

- 3-Hydroxystanozolol-3TMS
- 4-Hydroxystanozolol-3TMS
- Stanozolol-1TMS
- Stanozolol-2TMS
- Boldenone-2TMS
- 19-Norandrosterone-2TMS
- 17-alpha-Methylandrostan-3-alpha, 17-beta-diol (2TMS)
- Methytestosterone-2TMS (ISTD)
- 3-Hydroxystanozolol-2TMS
- 4-Hydroxystanozolol-2TMS
- 4-Hydroxystanozolol-3TMS
- 3-Hydroxystanozolol-3TMS

Masses, TIC

1st Dimension Retention Time
2nd Dimension Retention Time
Positive Identifications were made for 4 illegal drugs: Methamphetamine, Dextroamphetamine, Amphetamine, and 3,5-Dimethoxyamphetamine.
• Automated SPME - GC x GC - TOFMS analysis results show that trace (ppb) levels of drugs from various classes can be detected in urine.

• The study achieved quantitative calibration linearity of 90% or greater over the concentration range from 10 to 1000ng/mL.

• The results of this study indicate that trace level screening of drugs in urine can be performed without sample derivatization providing accurate identifications by automated solid phase microextraction (SPME) coupled with GCxGC-TOFMS.
This research demonstrates that the integration of an automated sampling method (SPME) without sample derivatization coupled with GCxGC-TOFMS analysis provides an effective method for drug screening. Study results prove that GCxGC-TOFMS achieves the resolution, sensitivity, and mass spectral integrity to accurately identify trace levels of drugs in complex sample matrices.

Future research will include experimental designs to meet guidelines set for federal workplace drug testing set by the Department of Health and Human Service (SAMSHA) Substance Abuse and Mental Health Services Agency.
Analysis of Drugs of Abuse by Gas Chromatography-Time-of-Flight Mass Spectrometry

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Life Science and Chemical Analysis Centre
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Overview

• Time-of-Flight Mass Spectrometry (TOFMS)
  – Benefits

• TruTOF HT GC-TOFMS
  – System Overview

• Rapid Drug ID by GC-TOFMS (EI & CI)
  – Experimental
  – Detection of Drugs of Abuse on Cotton Swabs

• Identification of a true unknown
Time-of-Flight MS Benefits

• Fastest Type of Mass Analyzer
  – Requires fast data acquisition system
  – Leco TruTOF HT: 80 Full Mass Range Spectra/s

• Ability to properly define narrow chromatographic peaks (HSGC)

• Delivers the data density needed for ‘True Signal Deconvolution’
  – Recommend 18-20 data points

• Full range mass spectrum is collected at all times without sacrificing speed or sensitivity….no need for SIM for best sensitivity

• Spectral Continuity (no spectral skewing)
Spectral Continuity

TOFMS  GC Peak  Scanning MS

[Graphs showing spectral continuity and mass to charge (m/z) with intensity and time (sec) axes]
TruTOF HT GC-TOFMS

System Features

• Benchtop Cabinet

• Sliding GC Base

• One-dimensional Separations

• Ion Source
  • EI and CI Options
  • Easy access for maintenance
  • Dual filament design (EI)
  • Ion source gate valve
Mass Analyzer

- Reflectron design
- Flight tube length: 1 m
- Discrete Dynode Detector
  - Low noise
  - Fast recovery time
  - Robust to air exposure
  - Linear response
  - Dynamic Range
Drug ID Method
## SPE Drug Mix Standard

<table>
<thead>
<tr>
<th>Component I.D. (In Order of Retention)</th>
<th>Molecular Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Amphetamine</td>
<td>135</td>
</tr>
<tr>
<td>Methamphetamine*</td>
<td>149</td>
</tr>
<tr>
<td>Butabarbital</td>
<td>212</td>
</tr>
<tr>
<td>Amobarbital</td>
<td>226</td>
</tr>
<tr>
<td>Meperidine</td>
<td>247</td>
</tr>
<tr>
<td>Pentobarbital</td>
<td>226</td>
</tr>
<tr>
<td>Secobarbital</td>
<td>238</td>
</tr>
<tr>
<td>Phenylclidine</td>
<td>243</td>
</tr>
<tr>
<td>Glutethimide</td>
<td>217</td>
</tr>
<tr>
<td>Phenobarbital</td>
<td>232</td>
</tr>
<tr>
<td>Methadone</td>
<td>309</td>
</tr>
<tr>
<td>Amitriptyline*</td>
<td>277</td>
</tr>
<tr>
<td>Imipramine</td>
<td>280</td>
</tr>
<tr>
<td>Doxepin*</td>
<td>279</td>
</tr>
<tr>
<td>Cocaine</td>
<td>303</td>
</tr>
<tr>
<td>Methaqualone</td>
<td>250</td>
</tr>
<tr>
<td>Desipramine</td>
<td>266</td>
</tr>
<tr>
<td>Pentazocine</td>
<td>285</td>
</tr>
<tr>
<td>Codeine</td>
<td>299</td>
</tr>
<tr>
<td>Oxycodone</td>
<td>315</td>
</tr>
</tbody>
</table>
Initial Drug ID Experimental

SAMPLES:
  SPE Drug Mix Standard (Alltech)

SAMPLE INTRODUCTION:
  MPS2 Autosampler (Gerstel) with a 10 µL syringe
  Injection: 1 µL

GC: Agilent 7890 Gas Chromatograph
  Column: 10m x 0.18mm x 0.18µm Phenomenex ZB-DRG1
  Inlet: Split 10:1 @ 280°C
  Carrier Gas: 0.43 mL/min, Constant Flow
  GC Oven: 70°C (2 min hold), 20°C/min to 130°C, 30°C/min to 280°C
  MS Transfer Line: 280°C

MS: LECO TruTOF HT
  Ion Source: EI at -70 eV
  Ion Source Temperature: 300°C
  Spectral Acquisition Rate: 10 spectra/s
  Acquired Mass Range: 40-500 m/z

Instrument Control and Data Review: ChromaTOF version 4.3
TIC for SPE Drug Mix
TIC for SPE Drug Mix

Original Method Elutes all Analytes in Approximately 11.5 minutes
TIC for SPE Drug Mix

- Amphetamine
- Methamphetamine
- Butabarbital
- Pentobarbital
- Phencyclidine
- Glutethimide
- Phenobarbital
- Methadone
- Amitriptyline
- Methaqualone
- Codeine
- Oxycodone

Time (s)

250 300 350 400 450 500 550 600 650

TIC
TIC for SPE Drug Mix

Time (s)

Imipramine
Doxepin
Cocaine
Methaqualone
Desipramine
Pentazocine
TIC for SPE Drug Mix (Deconvoluted)

- Imipramine
- Doxepin
- Cocaine
- Methaqualone
- Desipramine
- Pentazocine

Time (s)

<table>
<thead>
<tr>
<th>TIC</th>
<th>234</th>
<th>58</th>
<th>182</th>
<th>235</th>
<th>195</th>
</tr>
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<tbody>
<tr>
<td>568</td>
<td>570</td>
<td>572</td>
<td>574</td>
<td>580</td>
<td>582</td>
</tr>
</tbody>
</table>
Deconvolution: Example
Deconvolution: Example

- Cocaine
- Methaqualone

Time (s)  573.5  574  574.5  575  575.5

TIC
Deconvolution: Example
Deconvolution: Example

Caliper

图书馆匹配 - 相似性929，"Cocaine"

图书馆匹配 - 相似性934，"Methaqualone"
Can We Go Faster?
Rapid Drug ID Experimental

SAMPLES:
SPE Drug Mix Standard (Alltech)

SAMPLE INTRODUCTION:
MPS2 Autosampler (Gerstel) with a 10 µL syringe
Injection: 1 µL

GC: Agilent 7890 Gas Chromatograph
Column: 10m x 0.18mm x 0.18µm Phenomenex ZB-DRG1
Inlet: Split 10:1 @ 280°C
Carrier Gas: ramped flow 0.43 mL/min to 2.0 mL/min
GC Oven: 70°C to 280°C @ 50°C/min, hold 1 min
MS Transfer Line: 280°C

MS: LECO TruTOF HT
Ion Source: El at -70 eV; Methane Cl at -140 eV
Ion Source Temperature: El at 300°C; Methane Cl at 200°C
Spectral Acquisition Rate: 20 spectra/s
Acquired Mass Range: El 40-500 m/z; Methane Cl 50-500 m/z

Instrument Control and Data Review: ChromaTOF version 4.3
We Can Go Faster….Much Faster!

Original Method Elutes all Analytes in Approximately 11.5 minutes, now 4.5 minutes!
Chemical Ionization Application

Peak True - sample "**SPE Mix @ 50ug/mL:13", peak 14, at 101.7 s

Library Hit - similarity 946, "Methamphetamine"

mw = 149

Peak True - sample "**SPE Mix @ 50ug/mL:13", peak 71, at 221.1 s

Library Hit - similarity 942, "Amitriptyline"

mw = 277

Peak True - sample "**SPE Mix @ 50ug/mL:13", peak 78, at 226.8 s

Library Hit - similarity 950, "Doxepin"

mw = 279
Chemical Ionization Application

Peak True - sample "**SPE Mix @ 50ug/mL:13", peak 14, at 101.7 s

Library Hit - similarity 946, "Methamphetamine"

Peak True - sample "**SPE Mix @ 50ug/mL:13", peak 71, at 221.1 s

Library Hit - similarity 942, "Amtriptyline"

Peak True - sample "**SPE Mix @ 50ug/mL:13", peak 78, at 226.8 s

Library Hit - similarity 950, "Doxepin"

Peak True - sample "**SPE Mix @ 50ug/mL (Methane CI):1", peak 11, at 101.7 s

MH+

Peak True - sample "**SPE Mix @ 50ug/mL (Methane CI):1", peak 32, at 221.5 s

MH+

Peak True - sample "**SPE Mix @ 50ug/mL (Methane CI):1", peak 38, at 227.3 s

MH+
Real World Applications

• Cotton swab samples received from a collaborating forensic laboratory.
  – Swabs were collected at various locations within a suspected drug house
  – Rapid drug ID method was employed to identify drug residues that may be present on swabs

• Characterization of “Incense”
  – Plant material labeled as Damiana Leaf and Mullein Leaf Ext.
  – Material said to have hallucinogenic effects when smoked
Cotton Swab Samples
ChromaTOF References

- References are created based on a standard with all peaks identified (NIST)
- Reference constraints are set by the user
- The reference is then added to the DP method for automated sample comparison
Swab Sample Preparation

- Solvent extraction of swabs and procedural blank
  - 10mL methanol
  - 20 min Sonication

- Filtration
  - Sample and blank filtered using 0.45 micron syringe filter disc

- Concentrate
  - Extract evaporated under nitrogen to 1mL

- Transfer to GC autosampler vials for analysis
Rapid Drug ID Experimental

SAMPLES:
SPE Drug Mix Standard (Alltech)  
Cotton Wipes from Suspected Drug House

SAMPLE INTRODUCTION:
MPS2 Autosampler (Gerstel) with a 10 μL syringe  
Injection: 1μL

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Column: 10m x 0.18mm x 0.18μm Phenomenex ZB-DRG1  
Inlet: Split 10:1 @ 280°C  
Carrier Gas: ramped flow 0.43 mL/min to 2.0 mL/min  
GC Oven: 70°C to 280°C @ 50°C/min, hold 1 min  
MS Transfer Line: 280°C

MS: LECO TruTOF HT  
Ion Source: El at -70 eV; Methane Cl at -140 eV  
Ion Source Temperature: El at 300°C; Methane Cl at 200°C  
Spectral Acquisition Rate: 20 spectra/s  
Acquired Mass Range: El 40-500 m/z; Methane Cl 50-500 m/z

Instrument Control and Data Review: ChromaTOF version 4.3
## Reference Comparison Results

### Peak Table (1)

<table>
<thead>
<tr>
<th>Peak #</th>
<th>Name</th>
<th>Match</th>
<th>Type</th>
<th>R.T. (s)</th>
<th>Expected Analyte R.T. (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>230</td>
<td>Cocaine</td>
<td>830</td>
<td>Match</td>
<td>227.8</td>
<td>227.9</td>
</tr>
<tr>
<td></td>
<td>Amphetamine/DoA</td>
<td>800</td>
<td>Not Found</td>
<td>94.2</td>
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<tr>
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<td>Methamphetamine/DoA</td>
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<td>Not Found</td>
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<tr>
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<td>Butabarbital/DoA</td>
<td>800</td>
<td>Not Found</td>
<td>165.6</td>
<td></td>
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<tr>
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<td>Amobarbital/DoA</td>
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<tr>
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<td>Meperidine/DoA</td>
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<tr>
<td></td>
<td>Pentobarbital/DoA</td>
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<td>Not Found</td>
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<td>Not Found</td>
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<td>Amtriptlyne/DoA</td>
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<td>Not Found</td>
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<tr>
<td></td>
<td>Imipramine/DoA</td>
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<td>Not Found</td>
<td>225.5</td>
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<tr>
<td></td>
<td>Doxepin/DoA</td>
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### Reference Spectrum - Reference "DoA", Analyte "Cocaine"

![Reference Spectrum](image)
Incense Extract Characterization
“Incense” Sample Preparation

• Weighed 0.5g dried plant material into 20mL Vial
  – Add 10mL pentane
  – Place in Ultrasonic bath for 20 min
  – Transfer pentane extract to autosampler vial for analysis
Incense Extract ID Experimental

SAMPLES:
“Incense”

SAMPLE INTRODUCTION:
Agilent 7683 Autosampler w/ 5µL syringe
Injection: 1µL

GC: Agilent 7890 Gas Chromatograph
   Column: 15m x 0.25mm x 0.25µm Rxi5MS (Restek)
   Inlet: Split 50:1 @ 250°C
   Carrier Gas: 1.5 mL/min, constant flow
   GC Oven: 40°C to 340°C @ 15°C/min
   MS Transfer Line: 320°C

MS: LECO TruTOF HT
   Ion Source: El at -70 eV; Methane CI at -140 eV
   Ion Source Temperature: El at 250°C; Methane CI at 200°C
   Spectral Acquisition Rate: 20 spectra/s
   Acquired Mass Range: El 40-550 m/z; Methane CI 50-550 m/z

Instrument Control and Data Review: ChromaTOF version 4.3
TIC for Pentane Extract of "Incense"
Spectra for Unknown

Peak True - sample "Mr. Smiley Extract:1", peak 95, at 1147.9 s

Peak True - sample "Mr. Smiley Extract (Methane Cl):3", peak 194, at 739.9 s
Structure of Unknown

JWH-018 (1-pentyl-3-(1-naphthoyl)indole)
Conclusions

• GC-TOFMS is ideal for Positive ID of Drugs of Abuse
  
  – Deconvolution capability increases sample throughput by reducing the need for total chromatographic resolution
  
  – Automated peak find algorithm reduces amount of time required of analyst
  
  – Reference function of ChromaTOF software reduces the chances for false positives or misidentifications.
  
  – TOF provides classical EI mass spectra and optional CI for mw confirmation, making structural elucidation of unknowns possible.
For More Information

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269-985-5714

Email: sepsci@leco.com
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