Evaluation of a Transportable Linear Ion Trap Mass Spectrometer for Rapid Seized Drug Screening

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ABSTRACT

With increasing seized drug casework submissions, there is a need to explore alternative methods to improve laboratory efficiency. This study evaluates the BaySpec Continuity™ transportable linear ion trap (LIT) mass spectrometer coupled with thermal desorption-atmospheric pressure chemical ionization (TD-APCI) for rapid seized drug screening. A validated library-based method identified controlled substances and cutting agents, achieving 100% correct identification in both blind and authentic casework samples. The method demonstrated sufficient selectivity and repeatability, even for isobaric compounds using tandem mass spectrometry (MS/MS).

INTRODUCTION

The growing number of seized drug casework submissions is leading to further backlogs and pressure on forensic laboratories to decrease turnaround times [1]. Although color tests can be used to rapidly screen seized drug evidence in the field, color tests have known limitations, including issues with accurately identifying controlled substances in mixtures [2]. These limitations have led to increasing interest in field-portable instrumentation, including Raman spectroscopy, Fourier transform infrared (FTIR) spectroscopy, and gas chromatography-mass spectrometry (GC-MS). Whereas Raman and FTIR spectroscopy are quick and non-destructive, these techniques struggle with detecting minor components in mixtures [3]. In comparison, mass spectrometry techniques offer improved sensitivity for minor component detection; however, GC-MS requires longer analysis time for chromatographic separation [4]. This study evaluates the capabilities and limitations of a transportable LIT mass spectrometer under controlled laboratory conditions. An internal library of common controlled substances and cutting agents was created, and a library-based alarm system was developed and validated for rapid seized drug screening.

MATERIALS & METHODS

Chemicals and Sample Preparation

The controlled substances and cutting agents analyzed in this study included cocaine, methamphetamine, heroin, fentanyl, caffeine, acetaminophen, pseudoephedrine, phentermine, phenacetin, and levamisole. All samples were prepared in a 49.9:49.9:0.2% methanol:water:glacial acetic acid solution for analysis. In addition to pure substances, five blind simulated and 10 authentic casework samples were prepared through solvent extraction using the same solvent described previously.

Instrumentation

A BaySpec Continuity™ transportable LIT mass spectrometer equipped with TD-APCI source with a TD heater temperature of 250 °C was utilized in this study. "Library selected ID list (MS, then MS/MS)" mode was used to collect full scan data in positive mode until a precursor ion exceeded a set threshold value, which is then fragmented to generate a product ion spectrum, triggering an alarm if the data matches a compound in the internal library.

RESULTS & DISCUSSION

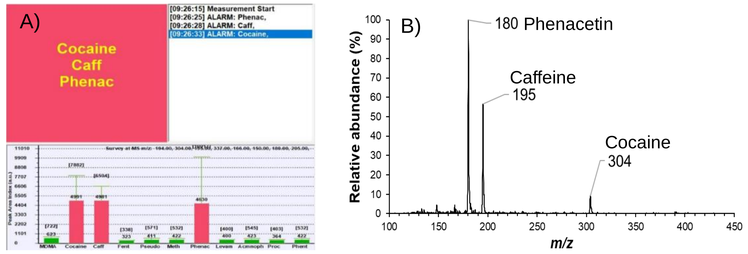

Figure 1. Examples of A) the library-based alarm system and B) the corresponding full scan spectrum for mixture #5 comprised of cocaine, caffeine, and phenacetin.

Table 2. Summary of compound LODs.

Compound	LOD (ppm)
Cocaine	15
Methamphetamine	10
Heroin	40
Fentanyl	10
Caffeine	2.5
Phentermine	7
Pseudoephedrine	30
Phenacetin	1
Levamisole	15

- Reliable and accurate identification was achieved for each pure compound and mixture in the validation study.
- The library-based identification results were repeatable within a day and reproducible across a week.
- The LOD is impacted by the ionization efficiency of the compound, as well as the efficiency of the isolation, fragmentation, and detection of product ions.

Table 3. Results of the authentic destroyed casework samples.

Authentic Samples	Screening Results	Correct Identification
1	Methamphetamine	✓
2	Cocaine	✓
3	Methamphetamine	✓
4	Cocaine	✓*
5	Methamphetamine	✓
6	Cocaine	✓
7	Cocaine	✓
8	Methamphetamine	✓
9	Methamphetamine	✓
10	Methamphetamine	✓

*Methamphetamine and procaine contamination detected

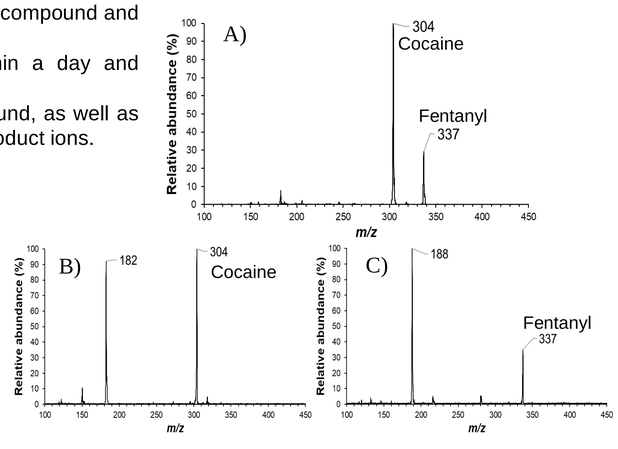

Figure 2. Exemplar mass spectra for blind sample #4 for A) the full scan spectrum, B) the product ion spectrum for cocaine, and C) the product ion spectrum for fentanyl.

- The library-based alarm system achieved a 100% correct identification rate for the controlled substance and cutting agents in the 15 blind simulant and authentic destroyed casework samples, even when methamphetamine and procaine contamination occurred.
- Product ion spectra were collected for each precursor ion within the blind mixtures and authentic destroyed casework samples.

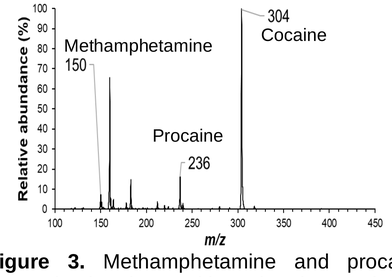

Figure 3. Methamphetamine and procaine contamination detected in authentic sample #4.

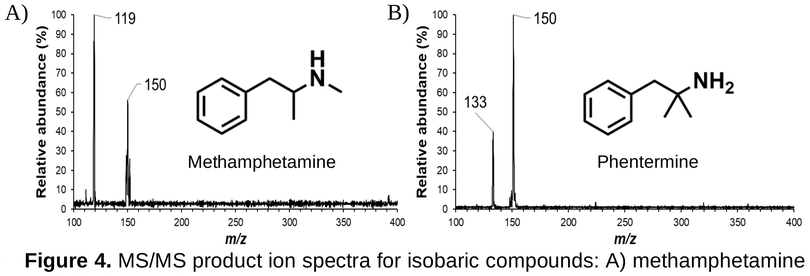

Figure 4. MS/MS product ion spectra for isobaric compounds: A) methamphetamine and B) phentermine.

- Methamphetamine contamination was likely from drug residue on the analytical balance during sample preparation [5].
- Differentiation of methamphetamine and phentermine based on the presence of product ions at *m/z* 119 and *m/z* 133, respectively.
- MS/MS capabilities provide a significant advantage for isomer differentiation, although only when unique product ions are formed.

MATERIALS & METHODS

Validation Study

Validation studies assessed the selectivity, repeatability, reproducibility, and limit of detection (LOD) of the library-based alarm screening method.

Table 1. Known mixture compositions for validation studies.

Mixture #	Compounds	Mixture Ratios
1	Heroin & Fentanyl	90:10
2	Cocaine & Levamisole	50:50
3	Methamphetamine & Pseudoephedrine	90:10
4	Methamphetamine, Caffeine, & Acetaminophen*	50:25:25
5	Cocaine, Caffeine, & Phenacetin	40:30:30

*Acetaminophen excluded due to poor ionization efficiency and insufficient product ions.

CONCLUSIONS

- Validated library-based alarm system screening method provides rapid and reliable identification of control substances even in the presence of common cutting agents.
- 100% correct identification of the controlled substances in 15 blind simulant and authentic samples.
- MS/MS enabled the differentiation of the isobaric compound methamphetamine and phentermine.
- Potential solution for improved laboratory turnaround times through higher-quality screening of seized drug evidence in a mobile laboratory environment.

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