Rapid Drug Screening Method by GC-TOFMS Analysis with the Pegasus® HT for 12 Drugs of Abuse in Under 5 Minutes

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Key Words: Pegasus® HT, GC-TOFMS, Rapid Drug Screening, Drugs of Abuse

1. Introduction

Crime laboratories have an immediate need for high throughput and definitive confirmation test methods that will relieve the on-going sample backlog burden. Illegal drug use worldwide is at an all time high. There is a crucial need for a fast and accurate analysis to positively identify suspected drugs in criminal investigations.

The capabilities and advantages of gas chromatography time-of-flight mass spectrometry (GC-TOFMS) are demonstrated with this application of non-derivitized samples showing a fast screening method for 12 different drugs of various chemical functionalities in 4.9 minutes. The benefits of utilizing the Pegasus® HT GC-TOFMS for drug identification analysis include acquiring highly sensitive full range non-skewed mass spectral information along with fast acquisition rates essential for high throughput analysis. This work demonstrates the ability of GC-TOFMS to increase laboratory productivity and efficiency while providing indisputable positive identifications for illegal drug analysis in criminal investigations. This work was conducted in collaboration with a local crime laboratory.

2. Experimental Conditions

Analytical results were generated with a LECO Pegasus time-of-flight mass spectrometer (TOFMS). The Pegasus GC-TOFMS instrument was equipped with an Agilent 6890 gas chromatograph and autosampler. LECO ChromaTOF® software was used for all acquisition control and data processing. A mixture of 12 different drugs from 4 different chemical classes was prepared as a standard for the rapid drug screen method development. The stock drug mixture was prepared in 5 mL of methanol from pure solid standards and then diluted (10:1) in methanol. The GC method injection port temperature was set to 260°C and a 1 uL split injection (10:1) was made. A 20 m x 0.18 mm i.d. x 0.18 µm film thickness, (Rxi-5ms, Restek Corp.) capillary column was used for the chromatographic separation. The GC was operated with helium carrier gas at a corrected constant flow of 2.0 mL per minute. The GC temperature program was set to an initial oven temperature of 125°C for 0.10 minute, followed by a temperature ramp of 70°C per minute, to a final temperature of 300°C held for 2.3 minutes, with a total run time of 4.9 minutes. The MS transfer line temperature was set to 260°C. The MS mass range was set at 40-450 amu with an acquisition rate of 10 spectra per second. The ion source chamber was held at 200°C and the detector voltage was set to 1850V with an electron energy of -70eV.

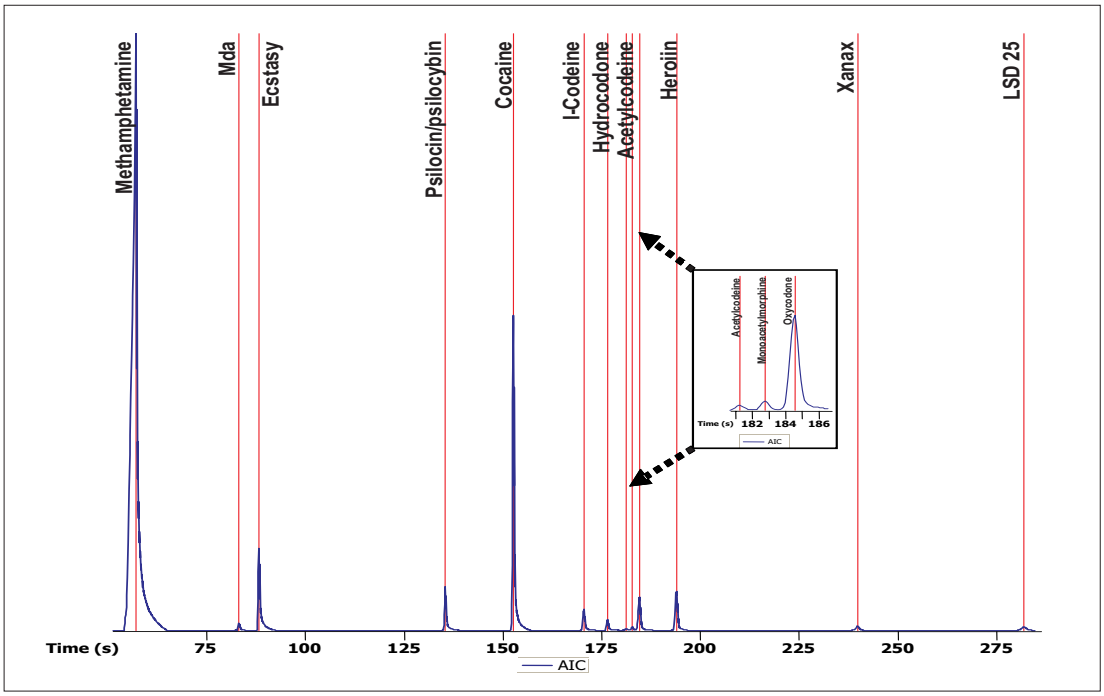

Figure 1. Figure 1 shows the Analytical Ion Chromatogram (AIC) for the rapid drug screen method of 12 drugs plus acetylcodeine in 4.9 minutes with an average similarity value of 870 out of 999. The inset shows 3 closely eluting peaks, acetylcodeine, monoacetylmorphine, and oxycodone.

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3. Results and Discussion

Figure 1 displays the chromatographic peaks for 12 drugs in the standard mixture plus acetylcodeine. The GC-TOFMS analysis for the rapid drug screen method was able to successfully identify all 12 components of the drug mixture in 4.9 minutes. Subsequently, a repeatability study was conducted on the same 12 component mixture by a sequence of 10 injections yielding reproducible results for all components. Mass spectral identification for all components was sustained in the repeatability study for all 10 injections. The 12 drugs of abuse plus acetylcodeine were identified with an average library match of 87% in less than 5 minutes. The GC-TOFMS rapid screen analysis method successfully overcame the analytical chromatographic challenges associated with several of the drug chemical classes. An uncomplicated, robust, and fast method was achieved by GC-TOFMS in 4.9 minutes confirming the value of the LECO Pegasus HT GC-TOFMS for rapid drug screening.

Mass spectral data in Figure 2 shows an example of the Caliper (A) total ion mass spectrum, the Peak True (B) deconvoluted mass spectrum, and the Library Hit (C) mass spectrum for the drug of abuse Oxycodone eluting at 184.5 seconds. The Peak True deconvoluted mass spectrum illustrates excellent corresponding fragment ions compared to the NIST Library mass spectrum with a similarity match of 893 out of 999.

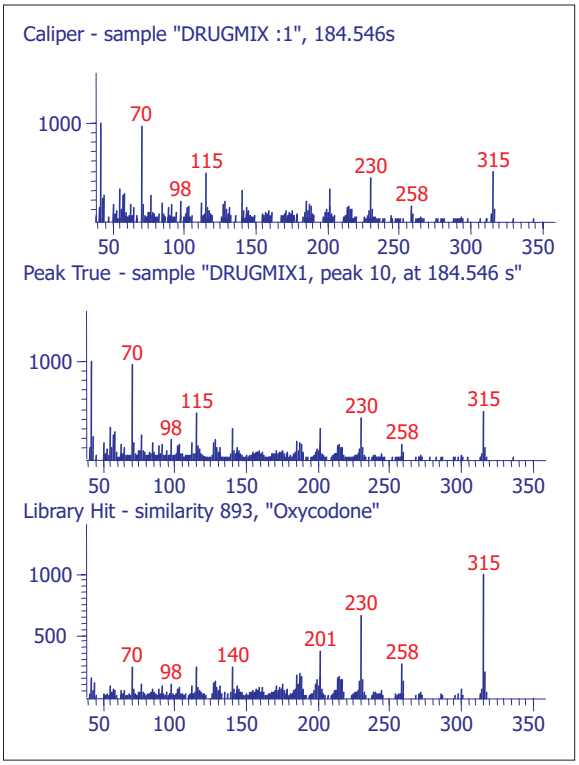

Figure 2. Figure 2 illustrates the Caliper (A) total ion mass spectrum, the Peak True (B) deconvoluted mass spectrum, and the Library Hit (C) mass spectrum for Oxycodone with a match similarity of 893 eluting at 184.55 seconds.

4. Conclusions

A successful and reproducible GC-TOFMS method was developed for rapid screening of illegal drugs from 4 different chemical classes in a single 4.9 minute analysis. All 12 target analytes plus acetylcodeine were confirmed by NIST MS library search with high similarity match scores without time consuming and costly sample derivitisation. The average similarity match score for the 12 component drug mixture was 87%. The benefits of utilizing the Pegasus HT GC-TOFMS for drug identification analysis include acquiring full range non-skewed mass spectral information along with fast acquisition rates essential for high throughput analysis. This collaborative effort with a local crime laboratory shows the advantages of GC-TOFMS to increase laboratory throughput while providing indisputable identifications for illegal drugs. This experimentation establishes that the LECO Pegasus® HT GC-TOFMS is an effective analytical tool in the fight against the rising worldwide drug abuse crime problem.

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