

FORENSIC TOXICOLOGY ANALYSIS

HIGH SENSITIVITY SCREENING FOR DRUGS OF ABUSE USING ALL-IONS ACQUISITION ON THE AGILENT 6550 QTOF



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Solution Note

Forensic Toxicology

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Abstract

A solution for compound screening with four dimensional identification using retention time, fragment qualifiers, accurate mass and isotope pattern matching.

Introduction

Confident identification of a compound can be achieved using the combination of All Ions data acquisition, in low and high energy MS domains, MS/MS spectral libraries stored in Agilent's Personal Compound Database and Libraries (PCDL) and Isotope Pattern evaluation of the parent compound.

This provides a quantitative and confirmatory screening workflow for the routine forensic toxicology screening laboratory capable of the highest sensitivity using High Resolution Accurate Mass (HRAM) technology.

The ability to de-convolute the high energy domain MS data using the MS/MS data from the PCDL is a unique feature of the Agilent Screening Solution. When this is used to generate a target screening method, subsequent analyses, using All Ions Acquisition can be processed directly in Mass Hunter Quantitative software using fragment ions as qualifiers and confirming the parent ion via isotope matching.

Using the Agilent 6550 Quadrupole Time-of-Flight LC-MS/MS system in combination with the Agilent 1290 Infinity Binary LC system sensitivities of tens of femtograms injected can be achieved. The exemplary compound used here is benzoylecgonine. The Agilent Forensic Toxicology PCDL contains over 9000 entries of which over 3000 have MS/MS spectra associated with them. These can be used to create specific PCDLs containing the compounds of interest for a particular screening workflow.



UHPLC – QTOF

- Agilent 1290 Infinity Binary LC system
- Agilent Eclipse Plus C18, 100 x 2.1 mm, 1.8 μm
- Agilent 6550 QTOF LC-MS/MS system
- Agilent Forensic Toxicology PCDL

Conclusion

Benzoylcegonine could be detected at 50fg injected on-column (figure 1) and fully qualified at 500fg injected. The presence of the fragments in the high energy MS domain can be used not only to confirm its presence but also as qualifying ions in MassHunter Quantitation software. The isotope pattern match i.e. accurate mass, isotope spacing and isotope abundance, can also be used to confirm identity (figure 2). Detection was linear over the range 50fg to 50 pg injected on-column (figure 3).

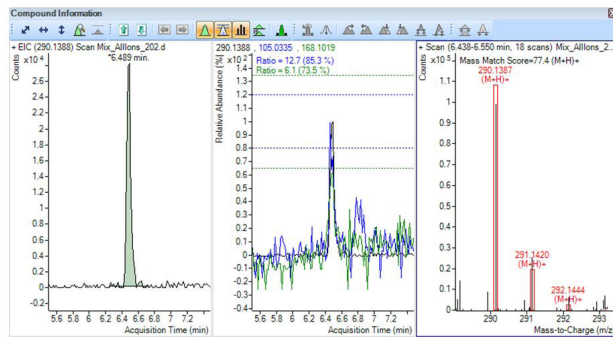


Figure 2. Compound qualifiers using Fragments, Accurate Mass and Isotope Pattern.

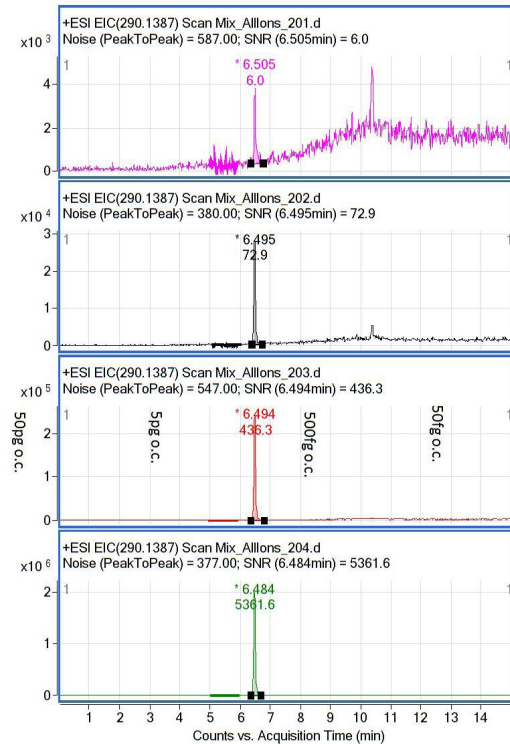


Figure 1. EIC of Benzoylcegonine at 50fg, 500fg, 5pg and 50pg on-column.

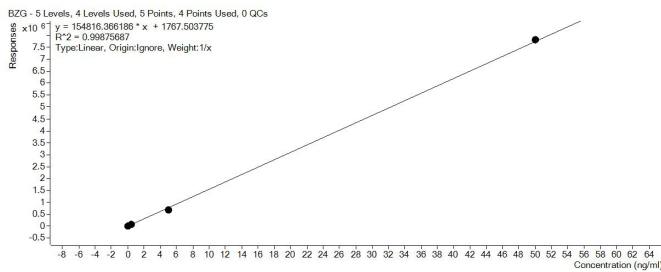


Figure 3. Linearity of detection of Benzoylcegonine.



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The Measure of Confidence



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