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Applikationsbericht

Extension of the Systematic Toxicological Screening Library for use with the Waters Nominal Mass Screening Solutions

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For forensic toxicology use only.

This is an Application Brief and does not contain a detailed Experimental section.

Abstract

This Application brief describes creating an additional library containing toxicologically relevant analytes that can be used for Systematic Toxicological Analysis (STA) with Waters nominal mass full scan screening solutions.

Benefits

An extension to the comprehensive systematic toxicological analysis library for use with either the Xevo TQD or Xevo TQ-S micro Mass Spectrometers has been created to bring the total number of analytes in the solution to 1200.

Introduction

Forensic toxicology laboratories require reliable screening techniques that can detect a wide variety of toxicants in highly complex biological matrices, such as ante and postmortem specimens. The original Waters systematic toxicological screening method used the Waters Alliance 2695 Separations Module in conjunction with the ZQ Single Quadrupole Mass Spectrometer.1 In 2009, this approach was migrated to the ACQUITY TQD System, to deliver the same comprehensive toxicological screening capabilities in half the time.[2]

The solution was further developed over subsequent years, to provide a full scan screening method and associated toxicology libraries, capable of screening for >950 drug substances and metabolites in 15 minutes. This method has been successfully and routinely used in toxicology laboratories worldwide.[3,4] Owing to the popularity of this methodology, in 2013, this solution was transferred to the ACQUITY UPLC I-Class/Xevo TQD System, and the release of the Xevo TQ-S micro in 2016 allowed for further evolution of this successful solution.[5,6]

Forensic toxicology laboratories are under great pressure to keep pace with the ever changing trends of the drug landscape with new psychoactive substances (NPS) or designer drugs being detected and characterized on a weekly basis. This highlights the importance of being able to increase the number of analytes in toxicology libraries to enable laboratories to detect more compounds.

Experimental

Test substances

Single analytes or mixtures of analytes were prepared in 5 mM ammonium formate pH3 at 2500 ng/mL.

Data acquisition

Data was acquired in full scan mode on the ACQUITY UPLC I-Class/Xevo TQD System using the STA method.[5]

Library creation

The acquired data was processed using the ChromaLynx Application Manager and a library was created in the NIST format using the built in ChromaLynx library creation tools.

Results and Discussion

A new library containing 244 analytes was created using the STA method on the ACQUITY UPLC I-Class/Xevo TQD System. This library was then converted for use with the ACQUITY UPLC I-Class/Xevo TQ-S micro System. This brings the total number of analytes in the Waters nominal mass full scan screening solution to 1200, increasing coverage for NPS and newer drug analogs whilst also expanding the applicability to sports doping analysis.

A library containing an additional 244 analytes was created. For each analyte the library contains the analyte name, molecular formula and retention time along with the mass spectra at multiple cone voltages in positive electrospray ionisation mode. The fragmentation pattern obtained for the psychedelic tryptamine 5-MeO-DMT ($C_{13}H_{18}N_2O$, retention time 2.6 minutes) is shown in Figure 1.

The library was converted for use with the ACQUITY UPLC I-Class/Xevo TQ-S micro System, which requires a different version of the acquisition method.[6]

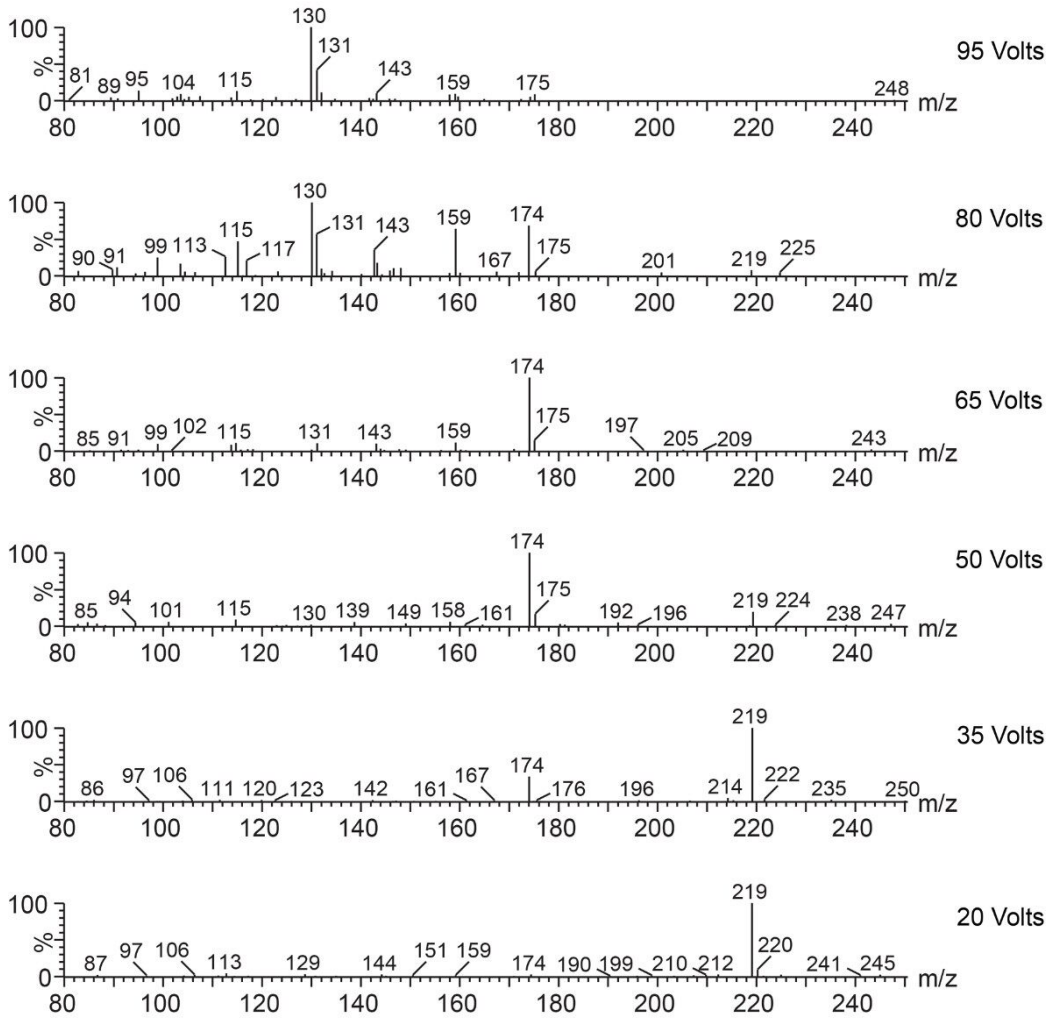

Figure 1. Fragmentation pattern for the psychedelic tryptamine 5-MeO-DMT across the six cone voltages used on the Xevo TQD.

Conclusion

A new library containing 244 analytes was created for use with the Waters nominal mass STA screening solutions to increase the total number of analytes in the forensic toxicology nominal mass screening solution to 1200. This library can be used on both the ACQUITY and Xevo TQD Mass Spectrometers in conjunction with the ACQUITY UPLC I-Class and the converted version can be used with the ACQUITY UPLC I-

Class/Xevo TQ-S micro System.

The additional analytes in the library increases the number of “designer” drugs and NPS such as designer benzodiazepines, psychedelic tryptamines, and fentanyl analogs that can now be detected using this screening method. The number of beta blockers, diuretics, steroids and receptor modulator drugs, which are of specific interest to sports doping laboratories, has also increased with this new release.

The easy to use ChromaLynx library creation tool allows customers to prepare their own libraries from either standard material or authentic samples. The additional library is formatted for immediate use and can be simply added to the customer’s existing library search method used by ChromaLynx to increase the number of analytes that can be detected using this screening method.

References

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5. Roberts M and Wood M. Forensic Toxicology Screening Using the ACQUITY UPLC I-Class System with the Xevo TQD. Waters Application Note. 720004602EN. 2013.
6. Lee R and Wood M. Systematic Toxicological Screening Using the ACQUITY I- Class/Xevo TQ-S micro. Waters Application Note. 720005661EN. 2016.

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Xevo TQ-S micro Triple Quadrupole Mass Spectrometry <https://www.waters.com/134798856>

ChromaLynx <https://www.waters.com/513759>

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