Bruker ToxScreener™

- A Comprehensive Screening Solution for Forensic Toxicology

UHR-TOF MS

Innovation with Integrity

ToxScreener - Get the Complete Picture

Forensic laboratories are frequently required to perform comprehensive screening of complex samples to identify drugs and other toxicants. This is a very challenging task due to the enormous number of analytes covered, their wide range of concentration and the complexity of sample matrices tested. Within the field of forensic toxicology, there is high requirement for analytical certainty in the accuracy and completeness of the results, so as to ensure that they will stand up to scrutiny in a court of law.

In recent years, owing to the high level of specificity and sensitivity obtained from full scan exact mass data acquisition, the utilization of Quadrupole Time-of-Flight (QTOF) technology for forensic toxicology screening has increased. Furthermore, the ability to retrospectively interrogate data for unexpected compounds, or emergent new "designer" drugs has significantly increased the uptake and adoption of this technology.
The application of QTOF technology for toxicological drug screening therefore offers forensic toxicologists a comprehensive solution for both targeted and non-targeted screening workflows. However, in order to realize this benefit, it is essential to have access to a high quality accurate mass reference database supported by powerful data processing software for cross referencing experimental observations.

The Bruker ToxScreener™ solution is designed specifically for use with Bruker QTOF mass spectrometers to enable comprehensive targeted forensic screening and confirmation of drugs and other toxicants in human body fluids, whilst delivering maximum confidence in the end result. The solution minimizes method development time for toxicological screening and is supplied with complete analysis protocols for the chromatographic and mass spectrometric analytical steps. The total analysis time including chromatographic separation and accurate mass detection is 20 minutes.
At the heart of the ToxScreener is a high quality forensic database that includes accurate mass and retention time information for over 1600 compounds of forensic relevance.*

ToxScreener Workflow

Prior to analysis, depending on the analytical requirements, blood serum or urine samples are prepared using LLE, SPE or protein precipitation. They are then injected onto a reverse phase binary gradient UHPLC- QTOF system for mass selective detection and confirmation.

The Bruker ToxScreener combines broadband CID (bbCID) QTOF data acquisition with the ToxScreener accurate mass forensic database and associated data mining software to bring the full power of exact mass screening to the forensic laboratory.

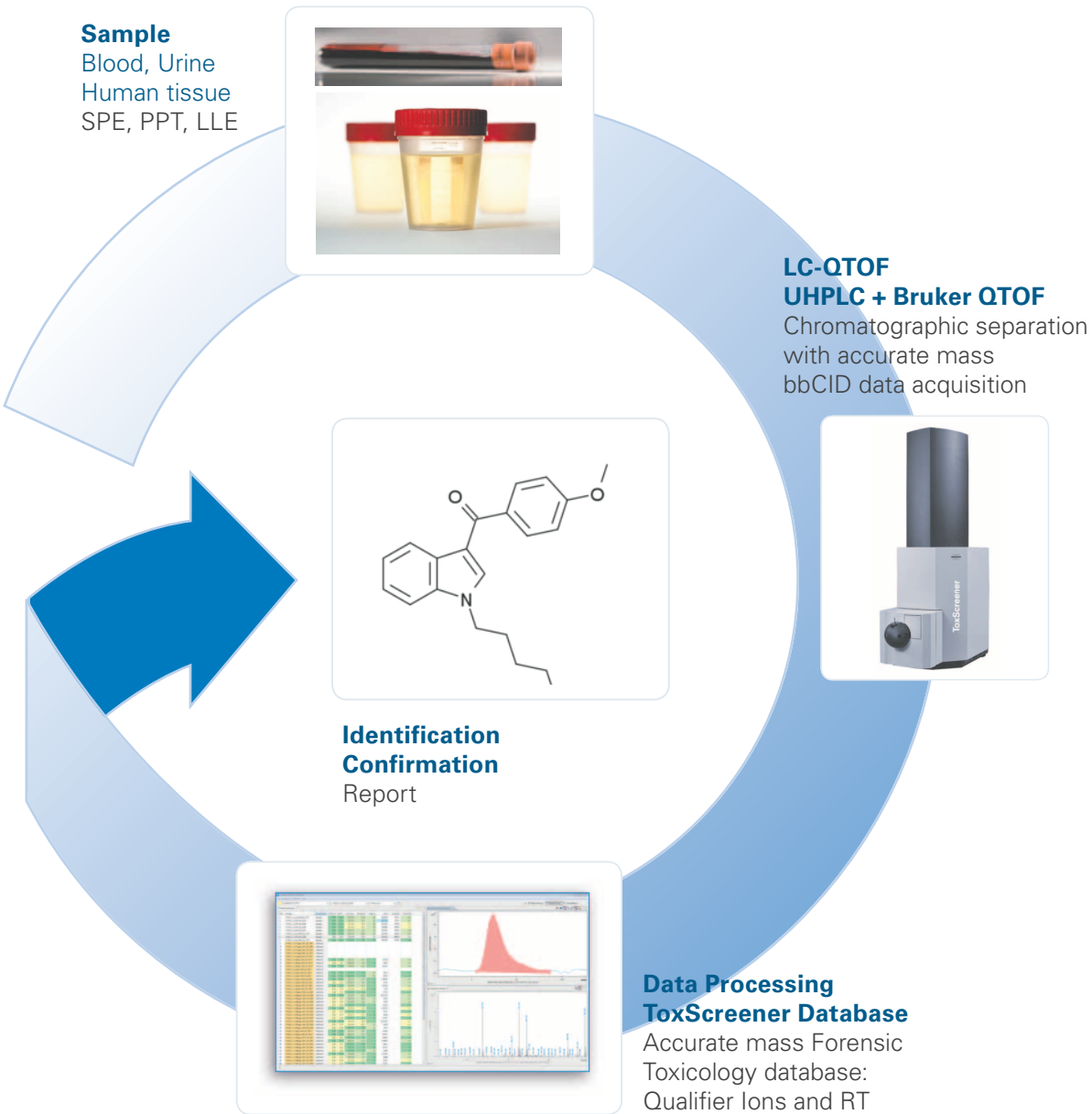

Fig.1: Schematic of Bruker ToxScreener Workflow

Broadband CID (bbCID) Data Acquisition

During the entire chromatographic separation step, the QTOF mass spectrometer rapidly and continuously cycles between TOF-MS and bbCID MS/MS resulting in the seamless collection of a comprehensive catalogue of precursor and fragment ion data in a single analysis.

The ability of QTOF instrumentation to collect 'all of the ions, all of the time' in both MS and MS/MS full scan modes results in a dataset that is complete and unrestricted. Once collected, the analyst can perform detailed targeted and / or non-targeted investigations if desired.

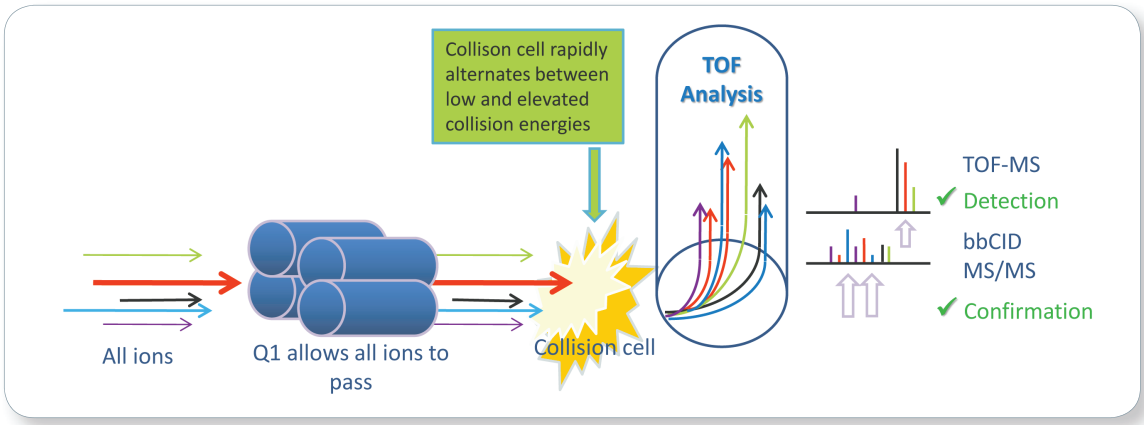

Fig.2: Schematic of Bruker broadbandCID (bbCID) data acquisition: The QTOF mass spectrometer rapidly alternates between two full scan accurate mass channels, one at low collision energy and the other at elevated collision energy.

Channel 1: Full scan data acquired at low collision energy. No precursor isolation and no fragmentation delivering exact mass precursor ion spectra (TOF-MS spectra).
Channel 2: Full scan data delivers at elevated collision energy: No precursor isolation with all ions undergoing fragmentation delivers exact mass of all fragment ions (bbCID spectra).

During data acquisition, simultaneous accurate mass measurement of pseudo molecular precursor ions and predetermined bbCID fragment ions that are characteristic to a specific compound (i.e. qualifier ions) provide enhanced levels of confirmation and so reduce false positive findings - see Figure 3.

Accurate mass measurement of intact precursor ions, true isotopic pattern and bbCID qualifier ions can be further extended to differentiate isobaric compounds including isomeric designer drugs. Figure 4 shows bbCID spectra differentiating two structurally isomeric synthetic cannabinoids, JWH-122 and JWH-019.

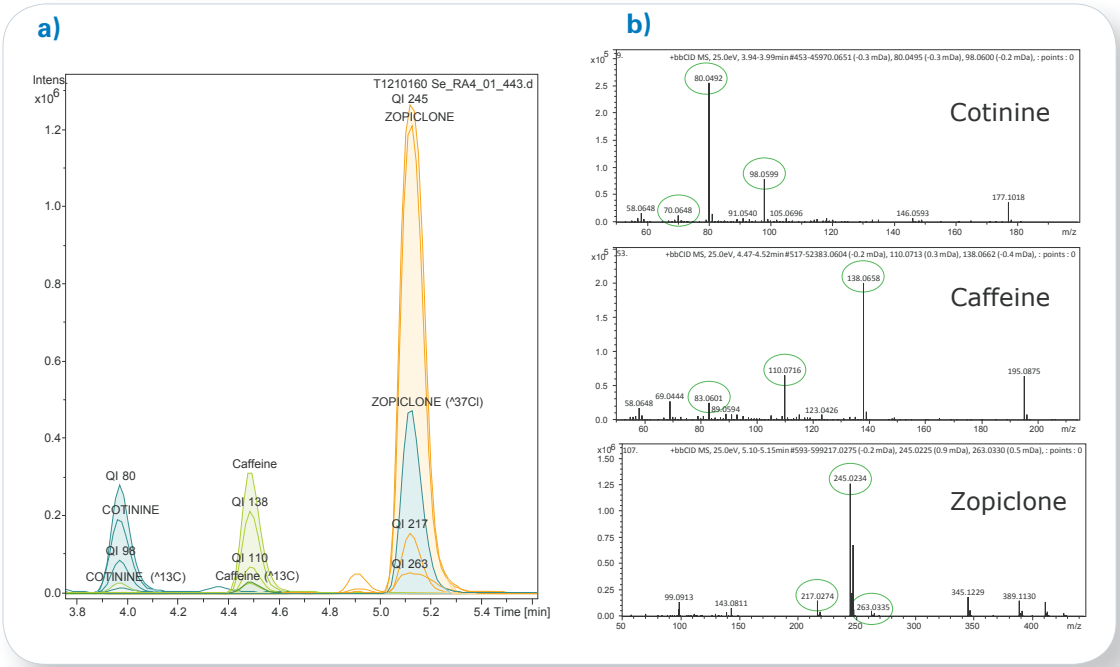

Fig.3: a) Chromatographic overlay of bbCID Qualifier (QI) Ion traces

b) bbCID spectra, Qualifier Ions circled in green

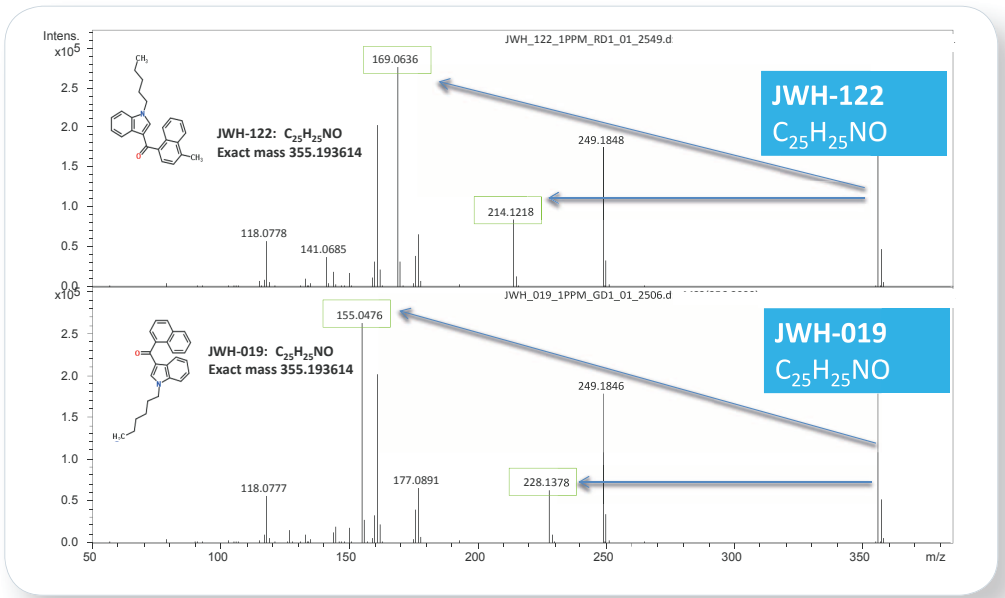

Fig.4: broadbandCID (bbCID) data acquisition differentiating two isomeric synthetic cannabinoids, JWH-122 and JWH-019. Their unique bbCID qualifier ions (highlighted in the green boxes) are used for unambiguous identification

ToxScreener Applications Kit

The ToxScreener applications kit incorporates a forensic toxicology accurate mass database detailing the exact mass of molecular ions, adducts, fragment ions as well as retention times that have been collected using an optimized UHPLC gradient to maximize confidence in identification. Also included within the applications kit are the analytical and guard columns, a test mix and all the necessary chromatographic and mass spectrometric parameters that are needed to perform the ToxScreener workflow.

Using accurate mass measurement, the ToxScreener forensic toxicology database allows you to screen and identify over 1,600 target analytes of forensic and toxicological interest in a single, short LC/MS/MS run. It is possible to add, remove and change the compounds included in the forensic database to meet the changing needs of your laboratory. Classes of compounds covered within the database include prohibited and therapeutic drugs as well as pesticides and designer drugs including cathinones and synthetic cannabinoids.

Ordering Information ToxScreener Applications kit: Part number 1827630
*Contact your local sales representative for a list of current compatible instruments.

For research use only. Not for use in diagnostic procedures.

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