Direct Sample Analysis Using a Thermal Extraction Ionization Source (TEIS) Combined with Mass Spectrometry

Technical Features and Attributes of the TEIS with a SCIEX QTRAP® System

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Mass Spectrometry (MS) is a widely used analytical technique for workflows requiring high levels of sensitivity and specificity. Historically, mass spectrometry has been predominantly used to support synthetic chemistry and pharmaceutical research but is nowadays becoming a standard in biotechnology, environmental research and forensic toxicology. However, traditional ion sources currently available on mass spectrometers require samples to be prepared in a specific way for introduction, limiting their utility for direct sampling workflows.

The ion source presented here overcomes the limitations of traditional ion sources and provides a way to rapidly detect low levels of analytes with little to no sample preparation. The source consists of a Thermal Extraction Ionization Source (TEIS)[1] operating with Thermal Desorption-Atmospheric Pressure Chemical Ionization (TD-APCI) coupled to a SCIEX Triple Quad™ or QTRAP® System. The technical features and attributes behind the combined system are herein described, showcasing its potential for rapid manual screening methods (with the option of sample automation) requiring minimal sample clean-up and no chromatography. The ease of use and versatility of the combined system enables confident trace detection of residues, substantially decreasing analysis time and false positives when compared to ion-mobility-based trace detection systems.[2]

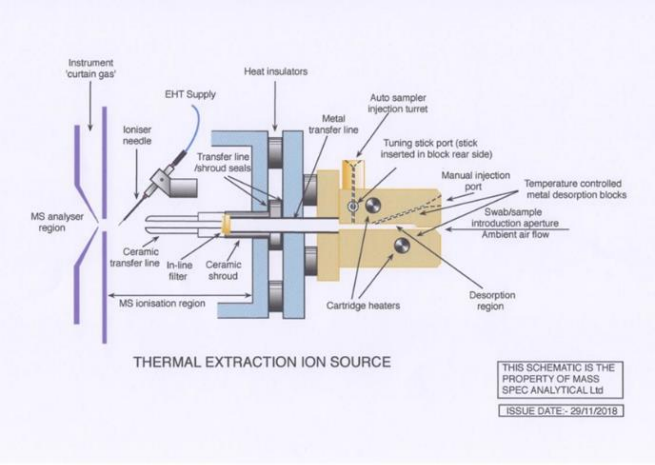

Figure 1: Schematic of the Thermal Extraction Ionization Source (TEIS). The source sits in front of the MS orifice and consists of two heated blocks, a transfer line and the APCI needle. This configuration provides direct sample introduction and real-time peak detection using the MS system.

Key Advantages of the TEIS Coupled to the QTRAP® System

- The Thermal Extraction Ionization Source (TEIS) provides direct sampling without sample preparation. When coupled to SCIEX mass spectrometers, the combined system offers the following advantages:
  - Samples can be directly introduced as swabs, vapors and liquids as the source is compatible with manual injection
  - Provides real-time peak detection of sample residues, generating confident identification within seconds
  - APCI affords sensitivity often in the low-picogram range
  - Self-purging source provides minimal carry-over between sample, with very little cleaning or maintenance
  - Reduces the need for chromatography through direct sample analysis
  - Requires very little consumables such as solvents and derivatives, reducing environmental impact
  - Easily coupled with most SCIEX Triple Quad or QTRAPSystems[3] for direct analysis and rapid identification, making it ideal for screening and confirmation applications
  - SCIEX systems are easy to use, rugged and versatile instruments designed to deliver a high level of sensitivity and robustness even for the most complex matrices
  - Full scan MS/MS achievable on QTRAP System for additional confidence in compound identification

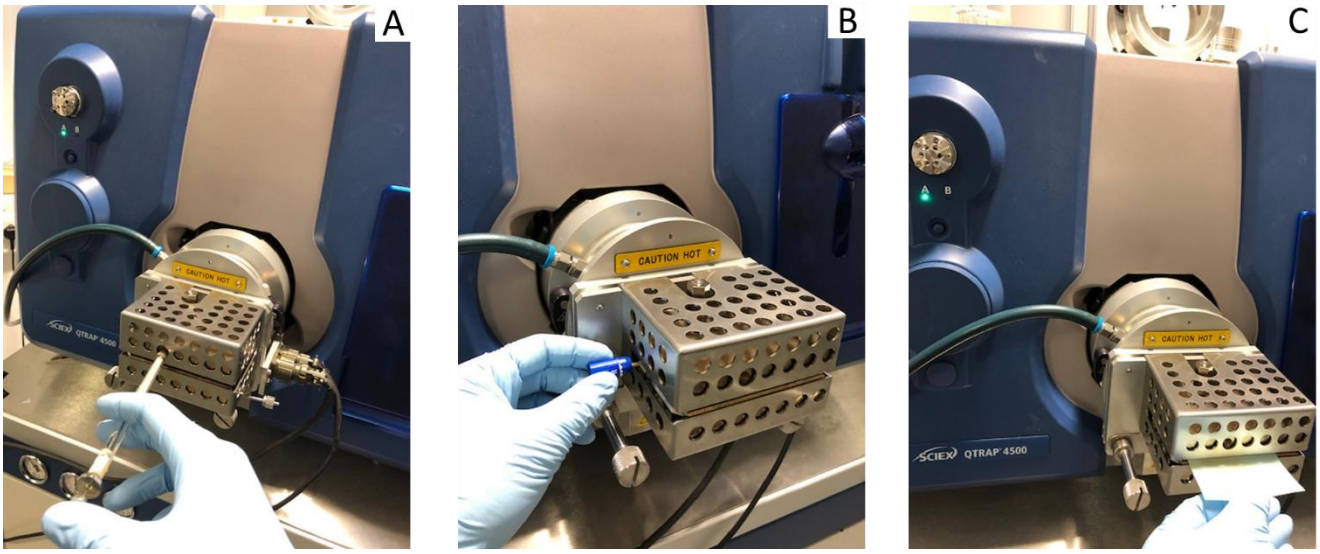

Figure 2: Different Sample Introduction Methods Available Using the TEIS. A) Manual injection using a syringe via the front injection port. B) Analyte residue sampling from a toothpick using the side injection port. C) Analyte residue paper swab sampling by inserting the substrate directly to the source between the two hot plates. Method development is typically performed using manual injection of reference standard solution via the front injection port.

Overview of Operation

The TEIS is based on Thermal Desorption - Atmospheric Pressure Chemical Ionization (TD-APCI) and consists of two parallel heated nickel-coated plates with a cavity between them, allowing ambient air to be continuously drawn between the plates and through a ceramic transfer line into the APCI source. The TEIS works by desorbing and/or volatilizing analytes from a surface or solvent using thermal desorption to convert the molecules into the gas phase. These gaseous molecules are then drawn through a ceramic transfer tube into the ionization region. Following APCI, the ions are detected by the mass spectrometer. Using the QTRAP systems with Analyst® Software[2], the user can quickly build streamlined detection methods based on the type of analyte or analysis required.

Technical Features

A schematic of the TEIS is depicted in Figure 1, showing the heated brass blocks, ceramic transfer line and APCI region in relation to the orifice. The source can be used for positive ion and negative ion detection of residues on surfaces, as well as for the detection of liquids and solids with minimal sample preparation. The TEIS operates at temperatures ranging from room temperature up to 325˚C which provides thermal desorption of a wide variety of analytes of varying volatilities. The high operating temperature and in-line filter promotes self-purging of the TEIS so that the combined system can cope with very complicated matrices without sample clean-up, with minimal carry-over between samples.

Configuration and Modes of Operation

The combined system allows direct analysis using the various sample introduction ports. Figure 2 shows the different sample introduction methods available using the TEIS. Manual liquid injections can be performed using a syringe via the front injection port (Figure 2A). A side injection port can be used for swab samples (Figure 2B) while other types of samples can be directly inserted into the source provided the surface is compatible with the operating temperature of the source (Figure 2C). A variety of sample substrates can also be used for direct analysis, including cotton, paper or even wooden swabs by simply inserting them directly into the heated region. Once the sample is inserted into the source, the detection of the analyte is nearly instantaneous.

Method development is performed in Tune Mode in Analyst Software. Here the user can easily switch between acquisition modes, tune method parameters, to develop an optimized sample analysis method. Once developed, the user can run methods in the more automated Acquire Mode and visualize in real time, using the Explore Mode, the thermal desorption profile of the MRM transitions used to specifically detect the target analytes.

Additionally, the design of the TEIS allows introduction of samples via the use of an autosampler, allowing hundreds of samples to be analyzed without the need for user intervention. This configuration can be used using a third party software for running fully automated batches in Acquire Mode in a high throughput fashion.

Functionality and Performance

The combination of the TEIS and the SCIEX QTRAP System provides the ability to easily develop high specificity methods, then perform rapid sample analysis robustly. Full scan capabilities of the QTRAP system allows both MS and MS/MS data to be acquired during method development to characterize the target analytes. This in turn allows the development and tuning of the specific MRM transitions for detection using the streamlined method optimization features in the Analyst Software.

During sample analysis, short dwell times can be used during MRM acquisition with minimal loss of sensitivity and performance to allow multiple analytes to be screened quickly. High dynamic range helps streamline acquisition, reducing the need for any re-analysis. MRM-triggered MS/MS workflows can also be used to collect full scan mass spectral data of the product ion for confirmation of identity. This can also be coupled with library searching for streamlined data processing. Using the TEIS with the QTRAP system allows for rapid sample analysis obtaining both MRM detection and MS/MS confirmation in a single analysis.

Streamlined Data Processing

When using the TEIS in combination to SCIEX mass spectrometers, the Explore Mode in Analyst Software allows the user to visualize the thermal desorption profile of the MRM transitions used to specifically detect the target analytes in real-time. The data acquired in Analyst Software can then be processed in MultiQuant™ or SCIEX OS Software, where the user can easily and quickly evaluate both the quantitation and screening results. In addition, these interfaces provide the ability to auto-generate customized sample reports. Compounds identified can be reported along with their amounts to quickly report the findings of the analysis. These features allow the user to automatically generate a comprehensive summary of the sample results, increasing laboratory throughput and freeing up operator time.

TEIS: The Ideal Ion Source for Residue Analysis

The TEIS is a versatile, reliable and easy to use ion source when coupled to a SCIEX System. Virtually any compounds amenable to thermal desorption and ionization by APCI, such as drugs, explosives, many pesticides and other environmental samples can be quickly analyzed and results can be generated nearly instantaneously. This novel method is ideal for contaminant and trace detection of explosives, drugs and other residues key in security screening applications, but can also be used in other application areas such as food, environmental, and forensic testing. When combined to a SCIEX System, the full system provides powerful direct analysis workflows for fast and confident detection of low levels of chemical residues.

References

1. For more information on the TEIS source, please visit www. msaltd.co.uk
2. D. S. Moore. Instrumentation for Trace Detection of High Explosives. *Review of Scientific Instruments.* (2004), **75**, 2499.
3. TEIS source is supported on most SCIEX Triple Quad and QTRAP systems, contact your local SCIEX sales representative for more information. Must using Analyst Software 1.7.1 or later.

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