Application Note

SICRIT®-MS: New Workflows in MS-based Analysis

Introduction

SICRIT (Soft Ionization by Chemical Reaction In Transfer) represents an innovative new ion source design enabling new modes and workflows for API mass spectrometry.
The patented SICRIT® soft ionization technology approach enables direct MS-based online gas-phase measurements (figure 1) as well as coupling with classical enrichment and separation techniques such as high performance liquid chromatography (HPLC), gas chromatography (GC), solid phase microextraction (SPME) or laser ablation (LA). Furthermore, automated sample preparation and processing can be implemented using PAL systems.

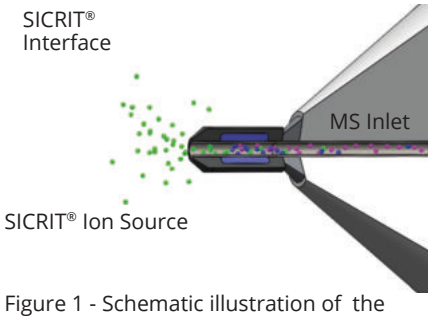

Figure 1 - Schematic illustration of the SICRIT® ion source design

Setup

SICRIT® extends the inlet of your MS and ionizes all molecules drawn in by your MS by means of a specially shaped cold plasma. The SICRIT® ionization technology can be adapted to any API mass spectrometer by individual interfaces, which can be easily installed on your MS inlet within few minutes. In combination with common sample separation techniques, the SICRIT® ion source presents an universal link between sample pre-treatment and MS-based sample analysis.

Figure 2 - Automated direct SPME-MS analysis using a PAL RTC sample preparation system and a SICRIT® SPME desorption module installed at a Thermo API MS inlet.

Fields of Application

The SICRIT® ion source implies several unique characteristics enabling new modes of sample processing and analysis.
The ion source acts as direct connector between chromatography and MS detector allowing to combine any chromatograph with any MS system. In this way, analyte molecules of a broad polarity range are softly ionized during transfer in the MS inlet. In consequence, SICRIT® is dedicated for powerful GC-soft-ionization-MS analysis, where MS instruments originally built for LC-MS applications can be utilized for GC-MS measurements. This new instrument combination provides MS data, which can be directly matched to the LC-MS data acquired on the same instrument. This approach will become a versatile tool for global and non-target sample investigation.

SICRIT® allows for new modes of MS-based sample analysis by shortening sample screening workflows and increasing the analytical power of GC-MS measurements.

For low-flow LC-MS (micro-, nano-LC), the SICRIT® ion source presents a viable solution for analysis of nonpolar analytes which can't be ionized with ESI and where APCI is not applicable due to the low flow rates.
Thinking of high-throughput screening (HTS) purposes, fast SICRIT®-based SPME-MS sample pre-screening without separation can be easily integrated in the automated routine HTS workflow and provides sufficient information to efficiently reduce the sample throughput which afterwards runs through the elaborate run.

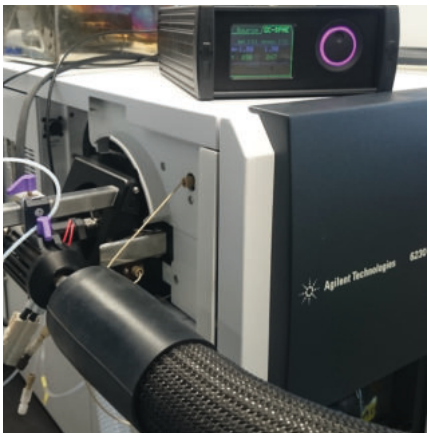

Figure 3 - SICRIT® GC-MS setup with transfer line attached to an Agilent TOF system.

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SICRIT® Measurement Examples

To illustrate the potential of the SICRIT® technology, representative examples of different analysis approaches are given. Screening of samples with direct SPME-MS is one of the designated application fields for SICRIT®. Thus, thermal desorption of SPME fibers and direct coupling to the API MS inlet by the ion source was investigated in several studies. For example, water samples spiked with drugs were extracted with 65 µm PDMS/DVB fibers and analysed using a Thermo LTQ Orbitrap in full scan mode with a resolution of 30 000 (figures 4 and 5). Desorption was conducted using a heating chamber with nitrogen (90% humidity) as carrier gas at 250 °C.

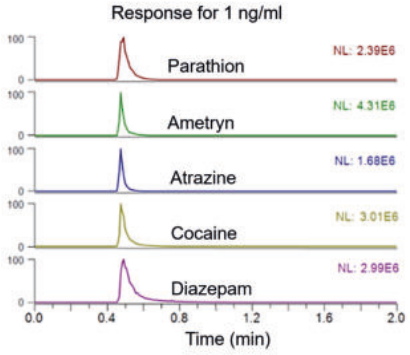

Figure 4 - Chromatogram of SPME-MS analysis of drugs in water samples at a concentration of 1 ng/mL after extraction for 5 min.

With this approach and a short extraction time of 5 minutes at RT, quantitative analysis with LODs in the low pg/mL range could be achieved.

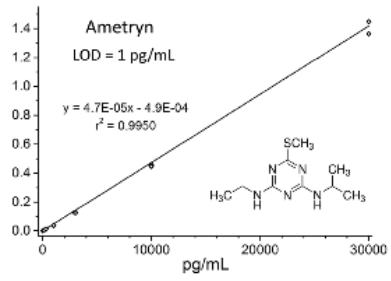

Figure 5 - Direct SPME-MS calibration of ametryn at a Thermo LTQ Orbitrap system.

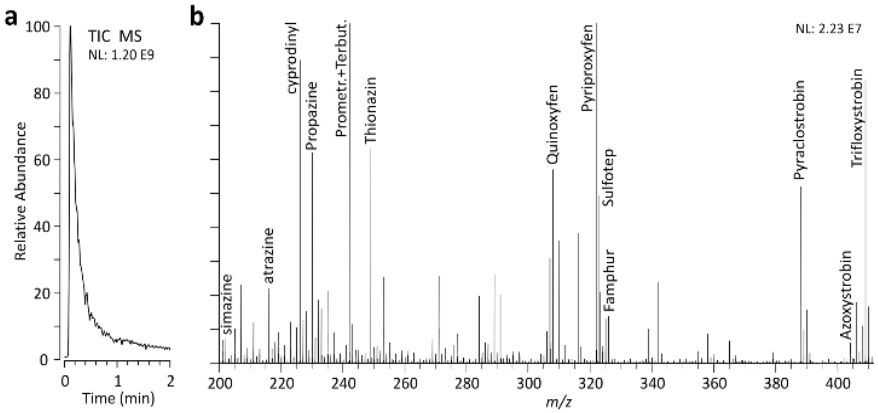

Figure 6 - TIC-MS (a) and high-resolution mass spectrum of direct SPME-MS of a mix of pesticides at a concentration of 10 ng/mL in grape juice after extraction for 20 min (b).

To elucidate the potential of the direct SPME-MS approach, also samples with more complex matrix composition were analyzed.
Therefore, grape juice samples were spiked with a pesticide mix and extracted for 20 minutes using PDMS/DVB fibers. After extraction, the fibers were rinsed in HPLC-grade water before desorption. Analysis was performed at a Thermo LTQ Orbitrap in full scan mode with a resolution of 30 000. Due to the variable pesticide structures, the observed LODs ranged from low pg/mL to low ng/mL, revealing RSDs below 10%.
Hence, direct coupling of SPME-MS by use of SICRIT® ion sources is a viable alternative to common extraction and separation methods in MS-based trace analysis of complex matrices.

SICRIT® Advantages

- Combinable with HPLC, GC, SPME and LA
- Adaptable to all available API MS systems
- Adapter for PAL systems
- High sensitivity (sub-ppt)
- Broad ionization range (positive and negative mode)
- Online-Screening Capability

Acknowledgements

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Related Publications

Mirabelli, M.F.; Wolf, J.-C.; Zenobi, R. *2016, Anal. Chem.,* 88, 7252.
Mirabelli, M.F.; Wolf, J.-C.; Zenobi, R. *2017, Analyst,* 142, 1909.
Mirabelli, M.F.; Gionfriddo, E.; Pawliszyn, J.; Zenobi, R. *2018, Analyst,* 143, 891.

Further Reading

Technical Note

TN_01 SICRIT® : Soft Ionization by Chemical Reaction In Transfer

Product Notes

PN_02 SICRIT® SC-20X Ionization Set
PN_03 SICRIT® GC/SPME Module

Application Note

AN_01 Chemical Warfare Agents - Direct SICRIT®-MS Analysis
AN_02 Coffee Aroma Profiling – Direct SICRIT®-HR-MS

KW TN_03_03/18

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