

# GC soft ionization coupling to LC-MS with SICRIT® (Thermo LTQ Orbitrap XL)

## Summary

- Easy Plug & play connection of any GC with any LC-MS using SICRIT and the SICRIT® GC-SPME module
- Soft ionization and high sensitivity
- High resolution MS data for non-target analytics
- Use your existing LC-MS software for GC-quantitation

## Introduction

Due to historic reasons the world of mass spectrometry is still divided into GC-MS and LC-MS systems and users thereof. Even from the big manufacturers perspective these are separate “markets” that are addressed with individual instrumentation and software.

But: Wouldn't it be nice to have the best of both worlds? The unmatched resolving power of a GC-MS with its broad EI ionization range combined with the high sensitivity, spectral resolution and soft ionization of LC-MS systems?

With SICRIT® this wish becomes reality!

The SICRIT® (Soft Ionization by Chemical Reaction In Transfer) source bridges the gap between GC and LC-MS by direct interfacing the instruments resulting in GC-soft ionization-MS.

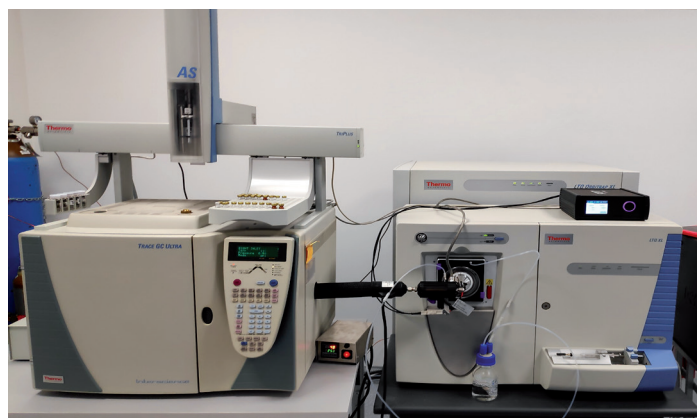


Figure 1 - SICRIT® coupling of a Thermo Trace GC Ultra to a Thermo LTQ Orbitrap XL.

## Experimental Setup

A Thermo LTQ Orbitrap XL was interfaced with a Thermo Trace GC Ultra measuring the SICRIT® positive tuning mix. This mix includes Trialkylamines with increasing chain length (see Table 2) and molecular masses between 143 and 269 amu.

Table 1 - Experimental setup and GC parameters.

Samples	SICRIT positive tuning mix in n-Hexane (1 ppb - 1 ppm)
Solvent	MS-grade n-Hexane (Sigma Aldrich)
Mass spectrometer	LTQ Orbitrap XL (Thermo Fischer)
SICRIT Plasma	1.5 kV, 15 kHz
GC	trace GC Thermo Finnigan
Liner	Restek, 5mm Splitless Borosilicate glass, deactivated, 105 mm
Column	Restek RXI-5ms, 30 m, 0.25 mm ID, 0.25 µm stationary phase
Inject volume	1 µL
Split ratio	Splitless
Carrier gas	Helium
Flow rate	Constant flow 2mL / min
Start temperature	40°C, hold for 0.5 min
Temperature ramp	40°C/min
Final temperature	280°C, hold for 3 min
Transfer line temperature	250°C

Quantitation was performed on exact mass traces (using a 5 ppm window). Peak picking and integration were performed with Thermo Xcalibur Software.

Table 2 - SICRIT® positive tuning mix with respective exact masses.

Compound	Sum Formula	Exact Mass
Tripropylamine	C <sub>9</sub> H <sub>21</sub> N	143.1702
Tributylamine	C <sub>12</sub> H <sub>27</sub> N	185.2138
Tripropylamine	C <sub>15</sub> H <sub>33</sub> N	227.2608
Trihexylamine	C <sub>18</sub> H <sub>39</sub> N	269.3077

## Results

In Figure 2, the extracted chromatogram (EIC) for 100 pg/amine on column is depicted. The four alkylamines show rising signals with increasing chain length, whereby separated peaks for the three tripentylamine isomers can be obtained.

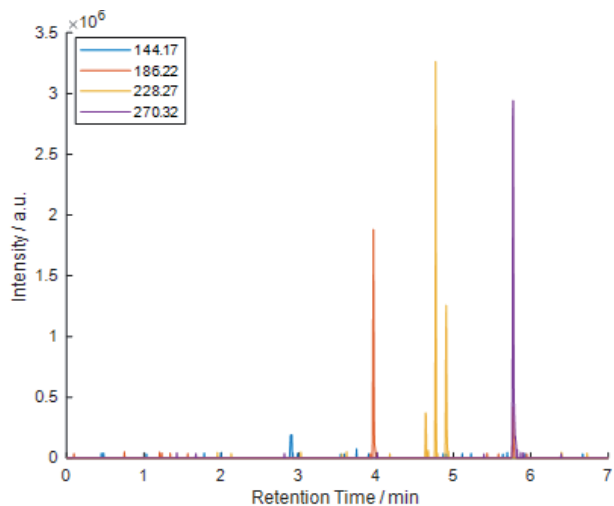


Figure 2 - EIC reconstructed GC-MS chromatogram of SICRIT® tuning mix solution (100 pg on column).

A full scan mass spectrum of tripentylamine is shown in Figure 3, illustrating the soft ionization of the SICRIT® source. The spectrum is clearly dominated by the signal of the  $[M+H]^+$  species, whereas fragment masses are barely formed.

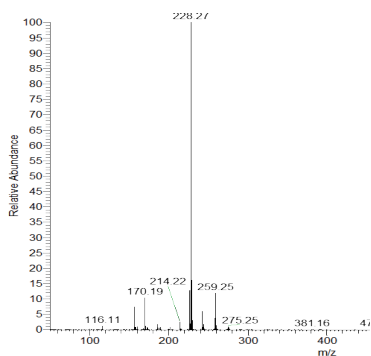


Figure 3 - Full Scan MS spectrum of tripentylamine, showing the soft ionization.

Repeatability of the GC-MS coupling was investigated by multiple consecutive injections and evaluation of the peak signal. The peaks of seven injections of the 1 ppm tuning mix standard were evaluated (see Figure 4). Low RSD values  $< 5\%$  confirm constant ionization performance and feasibility of Plasmion's novel GC-soft ionization-MS hyphenation.

One key feature of this coupling is the possibility to combine any GC to any LC-MS instruments. This allows for non-target applications realized by HRMS data. Using an Orbitrap system, high-resolved and accurate mass spectra ( $< 1$  ppm mass error) enable unambiguous identification of unknown compounds.

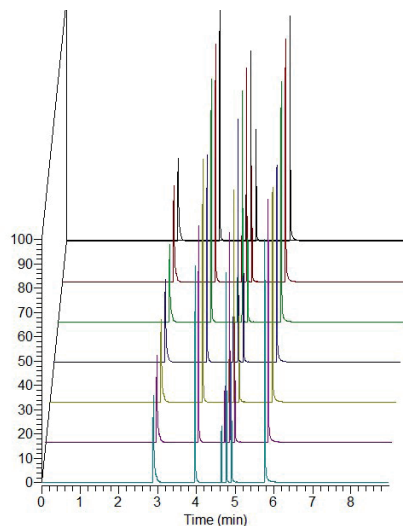


Figure 4 - Repeatability test showing 7 injections of 1ppm tuning mix.

Of course, SICRIT® coupling is also dedicated for quantitative target analysis, as exemplarily illustrated by calibration curves of tuning mix compounds in Figure 5 (1000 ppb – 1 ppb standards).

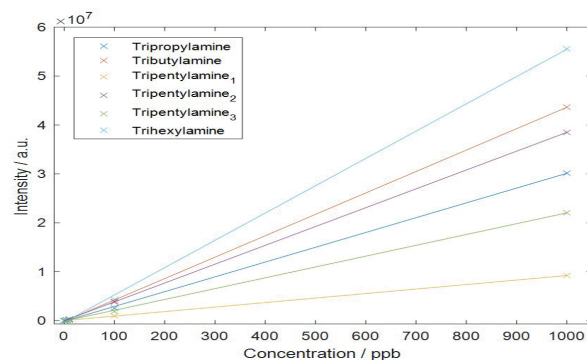


Figure 5 - Calibration curves for trialkylamine tuning mix ( $R_2 > 0.999$ ;  $n = 3$ ,  $m = 6$ ).

## Conclusions

SICRIT® enables the plug & play interfacing of LC-MS systems (here shown on Thermo LTQ Orbitrap XL) with any GC. For the investigated alkylamine mixture, the results show extraordinary performance:

- Dynamic range  $> 3$  orders of magnitude
- Sensitivity down to 1 pg on column
- Very soft and broad ionization range