



Direct MS Screening

Get results faster with SICRIT®

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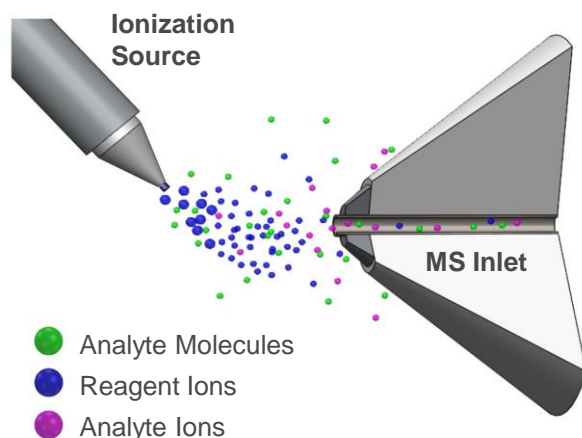
Dr. Jan-Christoph Wolf

04.05.2020



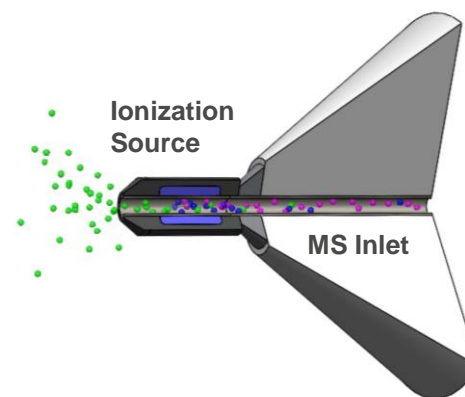
The patented flow-through geometry of the SICRIT[®] ionization source is new and unique

Conventional Ionization Technologies



VS.

SICRIT[®] Technology



SICRIT[®] Characteristics

- Simple extension of MS inlet
- Concentric dielectric barrier discharge
- Sample ionized during transfer into MS
- Soft ionization by proton transfer and UV light
- No consumables

With conventional atmospheric pressure methods, the **ions** are mostly **formed outside the inlet of an MS**. This implies that the substance to be analyzed (e.g. coffee) cannot be analyzed directly, but is usually "sprayed" into the MS in the form of a sample (liquid extract) via the ionization source

The SICRIT[®] (Soft Ionization by Chemical Reaction In Transfer) ionization source is **interfaced with the atmospheric pressure inlet of the MS** and ionizes every substance which is drawn into the MS by its inherent vacuum.

Reducing complexity of mass spectrometry in terms of preparation, execution and evaluation



Increased Sensitivity

The ionization within a closed chamber in extension of the inlet prevents columbic repulsion before the inlet and enables higher sensitivities



Enhanced Range of Analytes

Three simultaneous ionization mechanisms expand the range of detectable analytes, covering polar and non-polar components



No Sample Preparation

The ambient character of the ionization source allows to analyze solid, liquid, or gaseous samples in room air without sample preparation (direct screening)



Flexible Coupling

It is the only technique that provides a seamless coupling with all chromatography methods like GC, LC or SFC



No Fragmentation

The unique shape of the cold plasma enables a soft ionization of analytes and avoids fragmentation

Applications

- Direct screening
- GC/MS coupling
- LC/MS coupling
- SFC/MS coupling
- Laser ablation imaging

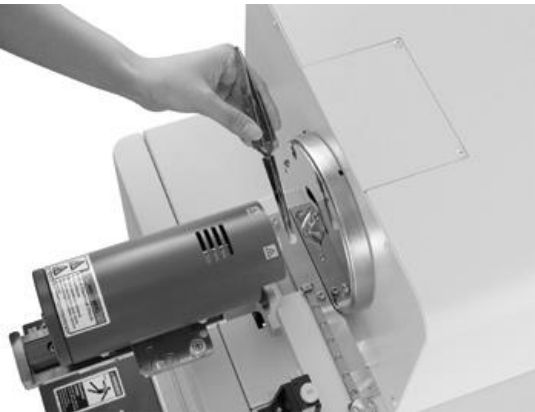
Currently, there are two prevalent methods dedicated for direct MS screening



Waters

ASAP Probe

Utilizes the heated nitrogen to vaporize the sample and a corona discharge for sample ionization



DART

Generates a plasma by glow discharge from the needle electrode in a helium gas stream



VS.



SICRIT®

Uses a dielectric barrier discharge to ionize molecules via a cold plasma as flow-through ionization

SICRIT® provides the possibility to perform screening with or without quantification

1

Screening without quantification

Some use cases in routine analyses can be supported by **direct screening**:

- Screening for **contaminations** like hazardous compounds or off-odors
- Identifying the **chemical composition** of unknown samples in a non-target approach
- Comparing different samples regarding their **relative exposure** to specific substances

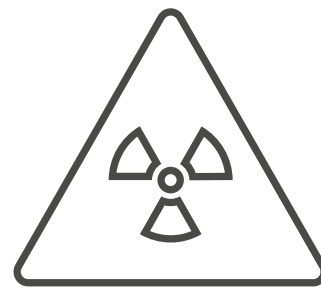
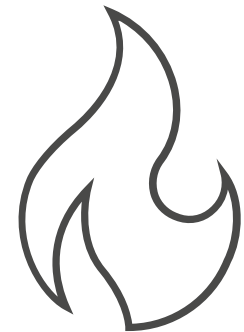
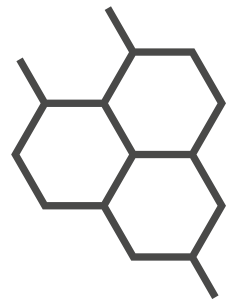
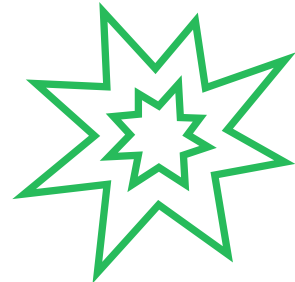
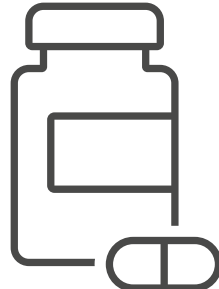
2

Screening with quantification

In other cases, **screening** is not sufficient as additionally the **quantification** of specific analytes may be required:

- Identifying the chemical composition of unknown samples and **determining the extent** of contamination in **absolute terms**

1 | Increasing importance of fast and reliable screening for harmful & hazardous substances



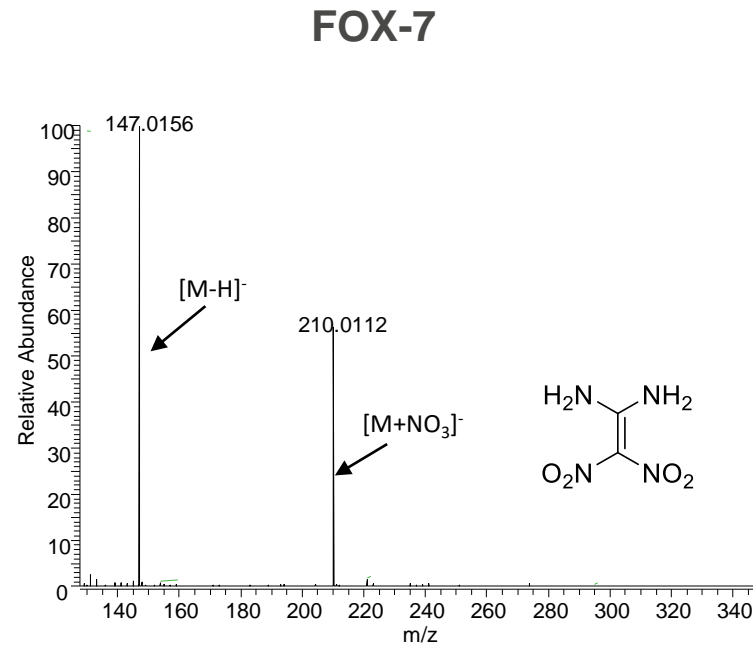
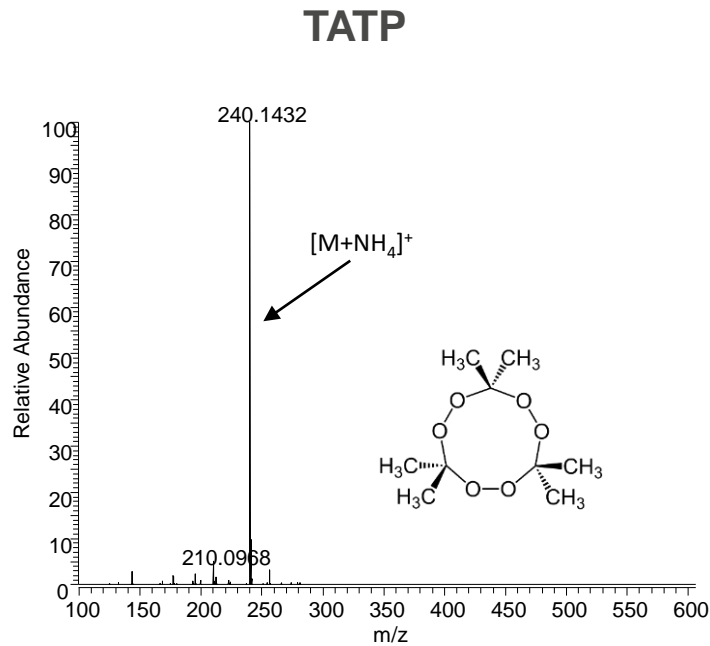
Background: Harmful & hazardous substances

In the case of harmful & hazardous samples **fast** and **sensitive** screening is essential

- Screening for drugs, explosives or toxins becomes more and more important
- Fast identification of contaminations with these compounds is crucial for our safety
- Especially **explosives** are by definition **instable** compounds and may disintegrate during analytics

1 SICRIT[®] enables to screen explosives and identify them within seconds

Mass spectra of selected explosives



Conclusion

- Seven different **explosives** have been investigated
- SICRIT[®] enables to identify different **explosives** by its molecular information
- Similarly fast **categorization of other harmful/hazardous substances** can be conducted

1 PFCA screening is becoming more important e.g. for textiles, however analysis is still challenging

Perfluorinated Carboxylic Acids (PFCA)

- **PFCA** is a substance group that features a **widespread use** in the context of different applications like
 - Water and oil repellents in fabrics and leather
 - Synthesis of fluoropolymers such as PTFE
 - Flame retardants
- In 2017, PFOA* and **PFOA-related substances** were **restricted** by REACH Regulation due to its cancerogenic and mutagenic effects
- In 2020, the production and distribution of **PFOA** will be **forbidden**

Current challenges in PFCA analyses

Quality control of textiles and other products marked as PFAS free becomes more important. However, current PFCA analyses are quite complex:

- **Tedious sample preparation** (e.g. cutting, extraction) and analyte enrichment
- **Analyte separation** is often **hampered** by adsorption effects and high blank values
- Current PFOA analysis **requires combination of LC and MS**

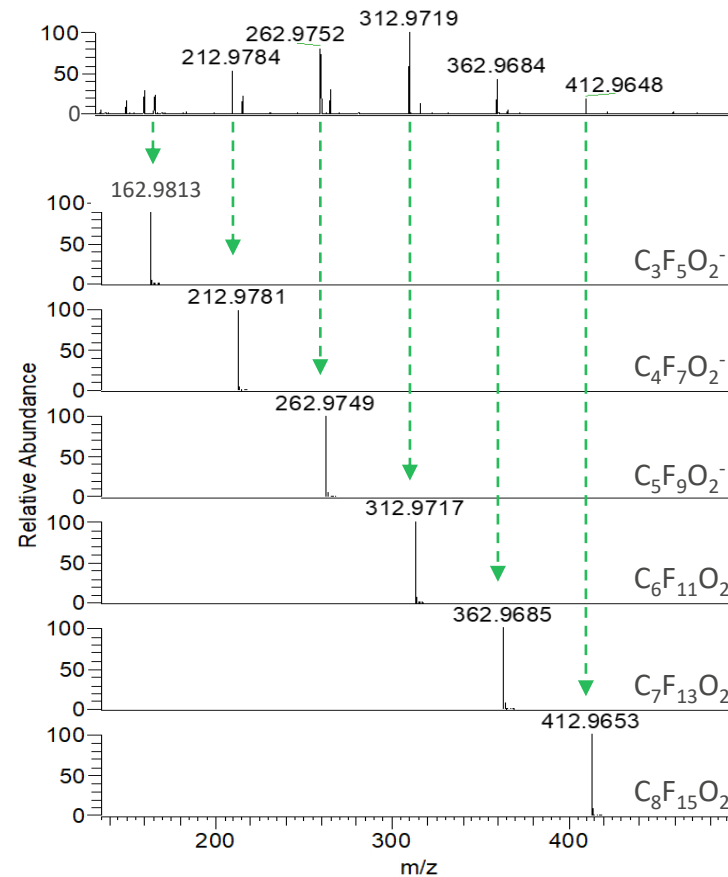
1 SICRIT[®]-MS allows for easy PFCA screening of any solid sample or coating solutions

Setup:

HRMS coupling with SICRIT and Thermo Fisher LTQ Orbitrap XL mass range 50 - 750 m/z, resolution of 30.000 FWHM



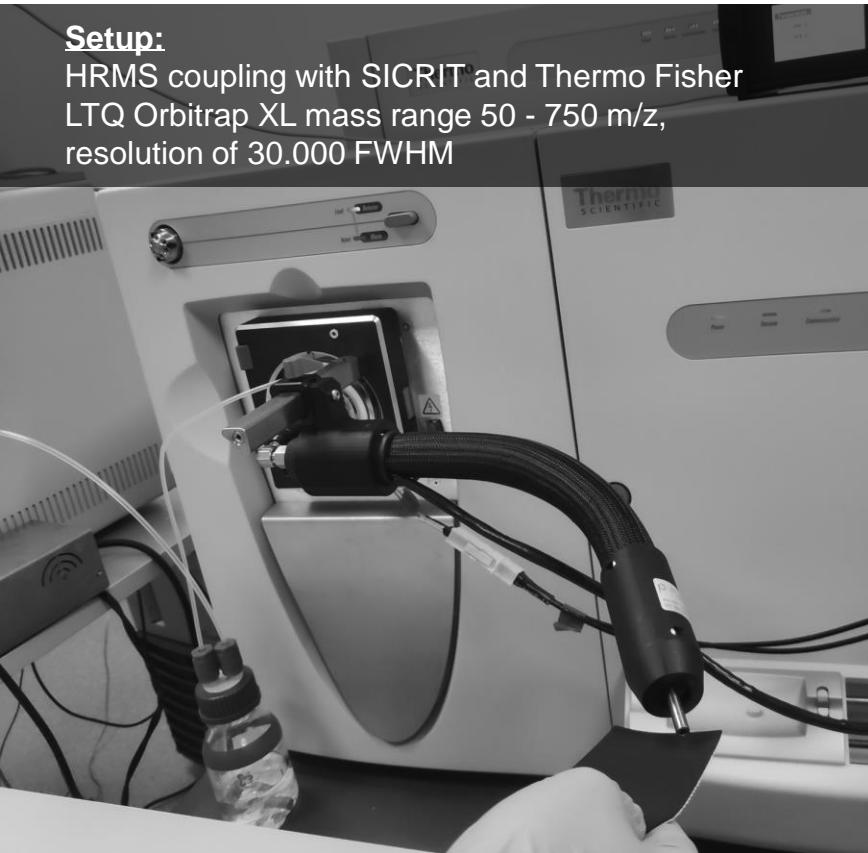
Spectrum and theoretical m/z of [M-H]⁻



Conclusion

- **Detect PFCA contamination in seconds** only by placing the sample in front of the SICRIT[®] ion source
- **No sample preparation** or analyte enrichment required

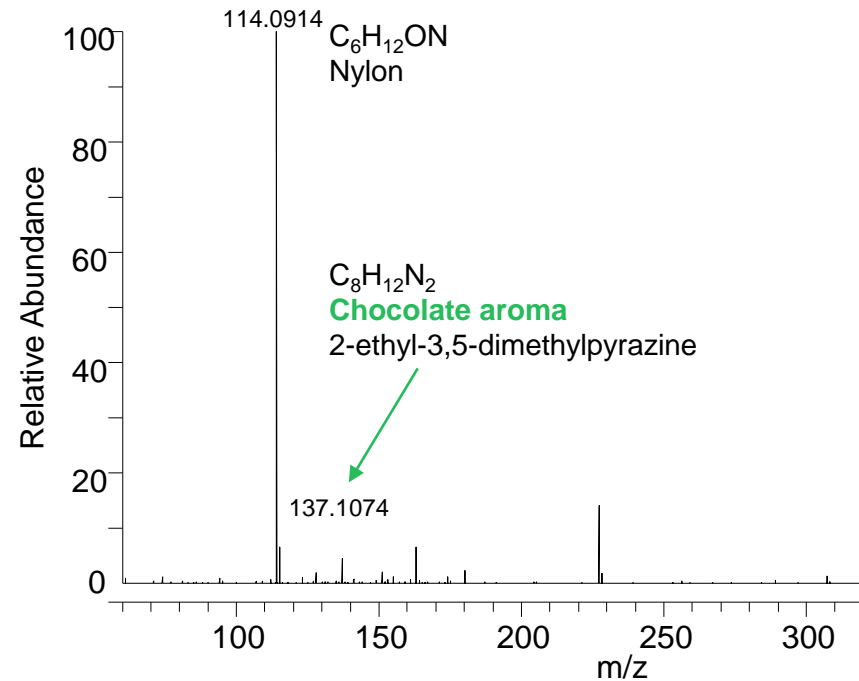
1 Generally, screening of textiles is getting more and more attention, e.g. in car interior analyses



Setup:

HRMS coupling with SICRIT and Thermo Fisher LTQ Orbitrap XL mass range 50 - 750 m/z, resolution of 30.000 FWHM

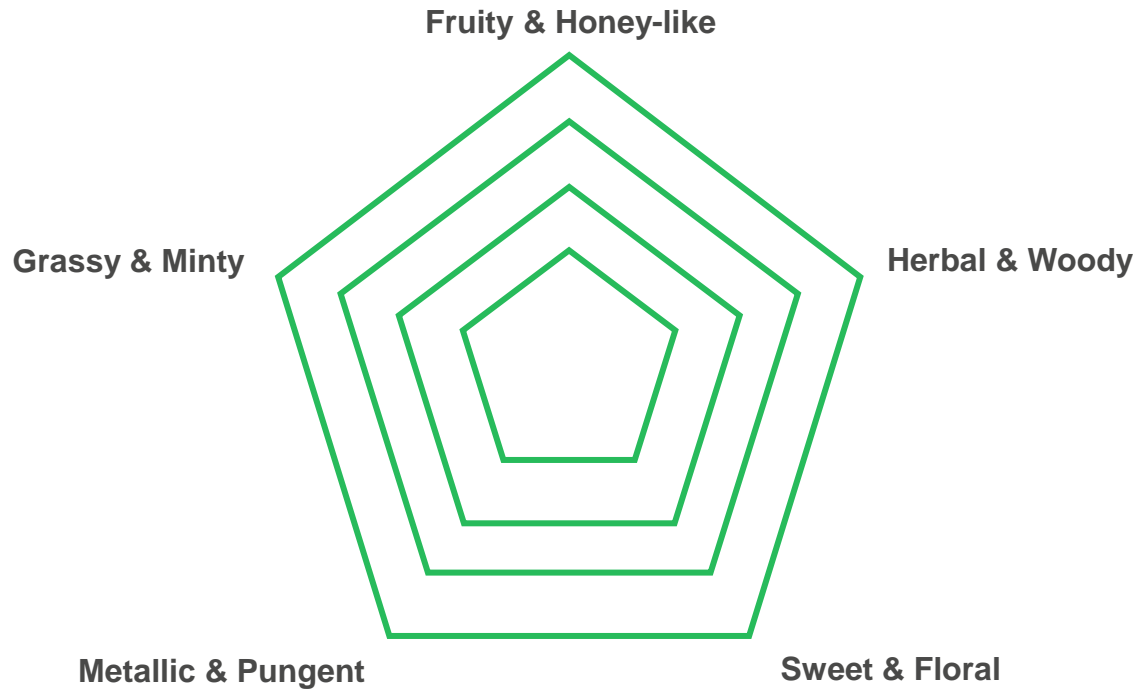
HRMS spectrum of artificial leather



Conclusion

- The leather was scented with 2-ethyl-3,5-dimethylpyrazine which causes a chocolate-like odour
- Additionally, other compounds related to leather material like nylon and PU could be identified

1 | Up to now, the most powerful tool in flavour analytics is the human nose



Current challenges in flavour analytics

Very volatile compounds need to be analyzed in **very low concentrations**

- Analyte separation and enrichment is necessary for technical detection of odors
- **Prevailing approaches** in R&D are human sensory panels and GC olfactometry that **have significant drawbacks**:
 - **Subjectivity** of human sensory panels **hampers** comparability in terms of **sensitivity and reliability** of detection
 - **GC-MS not capable** to identify all compounds, especially in **complex samples** like coffee or tee

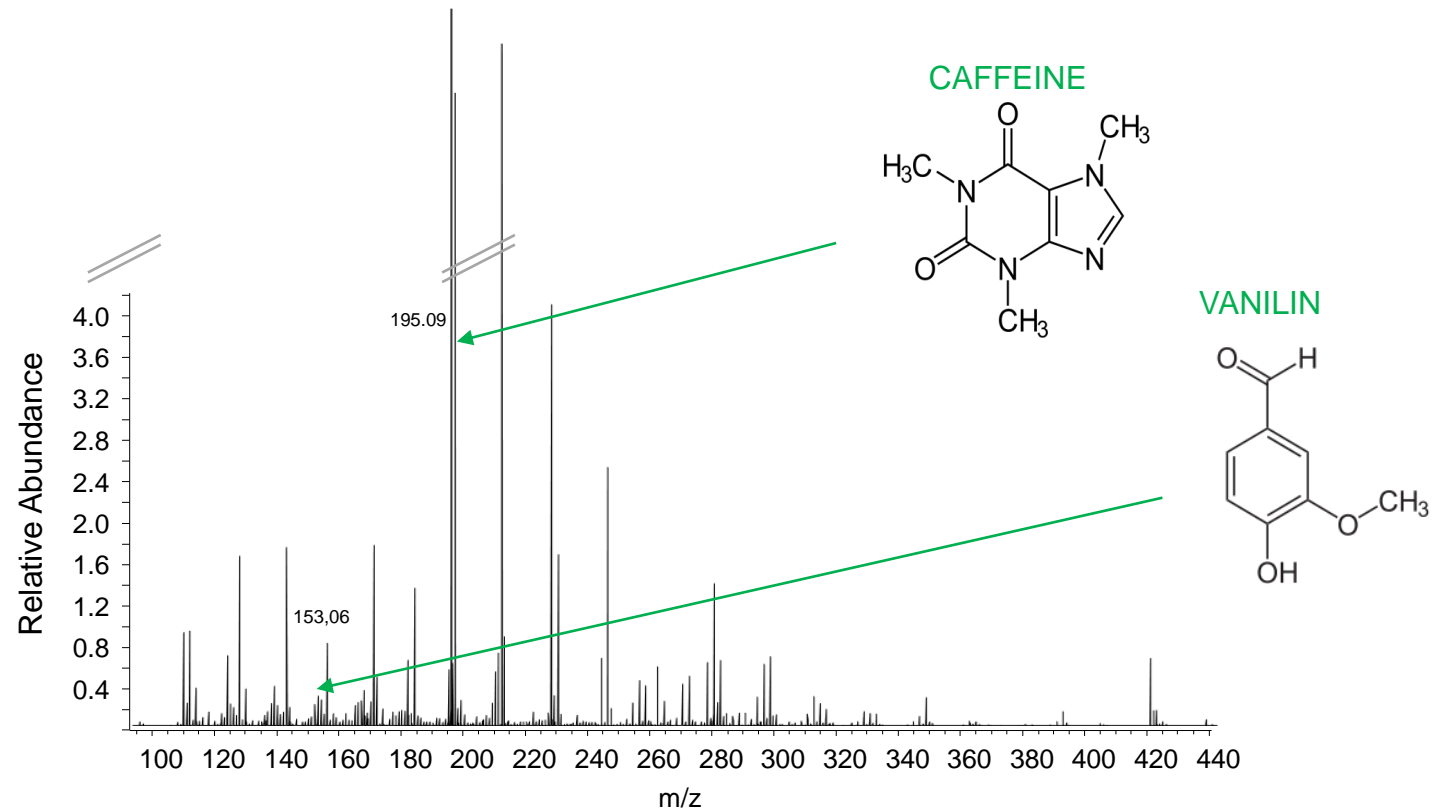
1 SICRIT[®] enables direct flavour and aroma analytics e.g. for the evaluation of coffee

Setup:

HRMS coupling with SICRIT and Thermo Fisher LTQ Orbitrap XL mass range 50 - 750 m/z, resolution of 30.000 FWHM Heated (100°C) support gas



HRMS spectrum of a single coffee bean

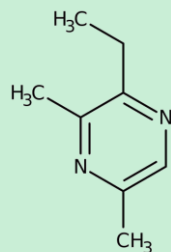


1 HR-SICRIT[®]-MS screening enables to detect and identify 500+ aroma compounds in parallel

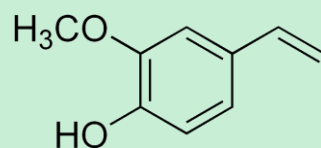
List of identified aroma compounds (excerpt)

Detailed in the following

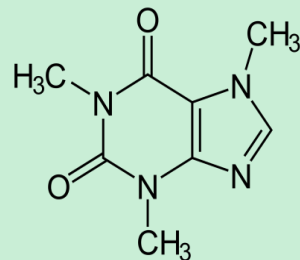
2-Ethyl-3,5-dimethyl-pyrazine



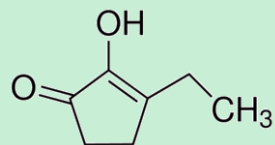
4-Ethylguaiacol



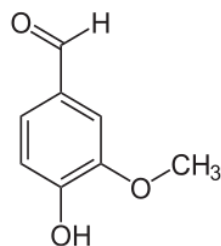
Caffeine



3-Ethyl-2-hydroxy-2-cyclopenten-1-one



Vanillin



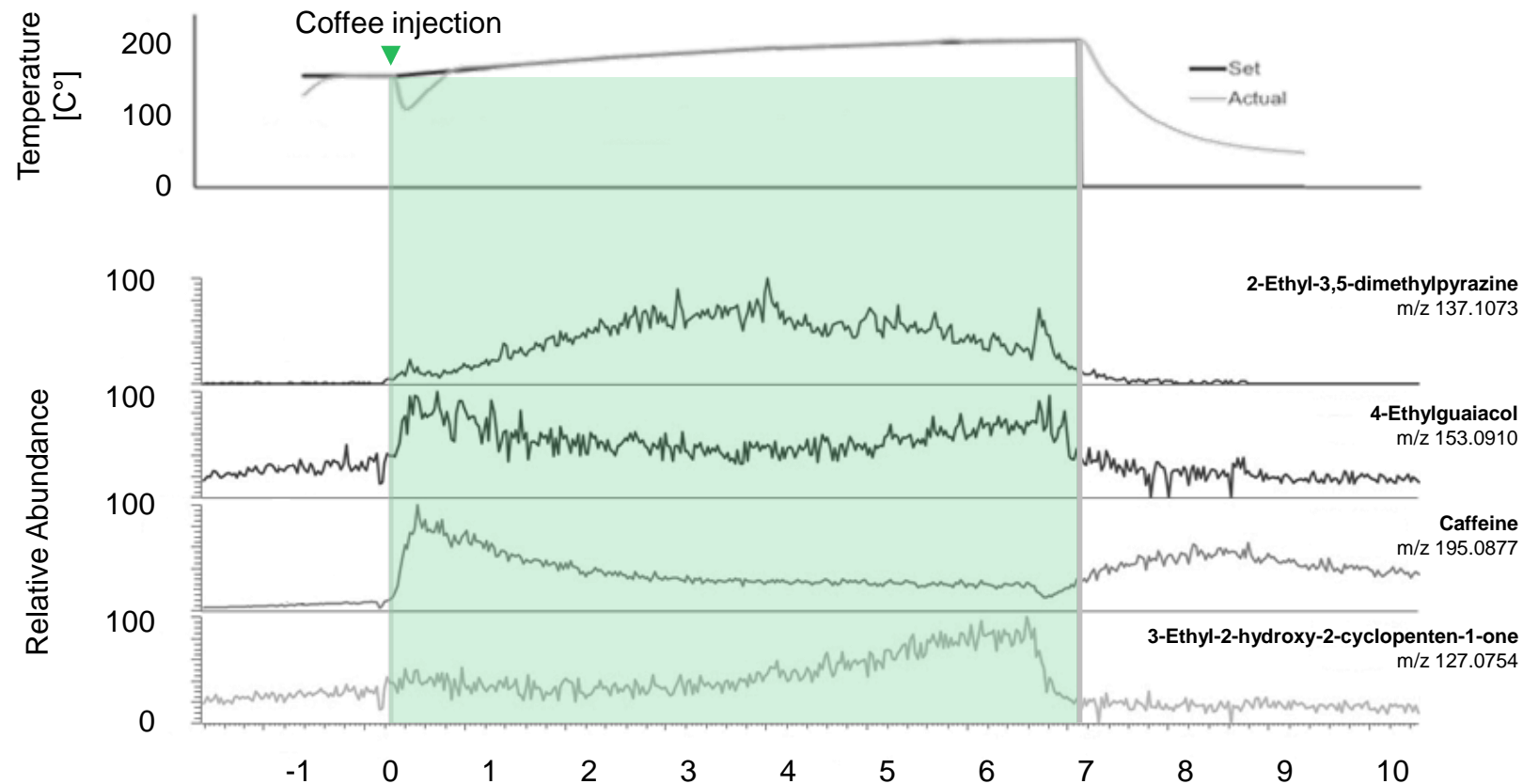
500+

Conclusion

- Non target **screening** of mass spectrum reveals more than **500 aroma compounds**
- **Distinct identification** by high mass accuracy
- **Matching** of flavour compounds (database) to MS data of coffee bean analysis **possible**
- **Detection of off-odours** (like Vanillin) directly possible

1 SICRIT[®] enables online monitoring of coffee roasting process with soft and broad ionization

Mass traces of selected aroma compounds*



Conclusion

- **Monitoring of aroma compounds during roasting process yields interesting insights** about their behaviours, e.g.:
 - Caffeine and 2-Ethyl-3,5-dimethylpyrazin (chocolate aroma) decreases with increasing temperature
 - 3-Ethyl-2-hydroxy-2-cyclopenten-1-one increases with increasing temperature

SICRIT[®] provides the possibility to perform screening with or without quantification

1

Screening without quantification

Some use cases in routine analyses can be supported by **direct screening**:

- Screening for **contaminations** like hazardous compounds or off-odors
- Identifying the **chemical composition** of unknown samples in a non-target approach
- Comparing different samples regarding their **relative exposure** to specific substances

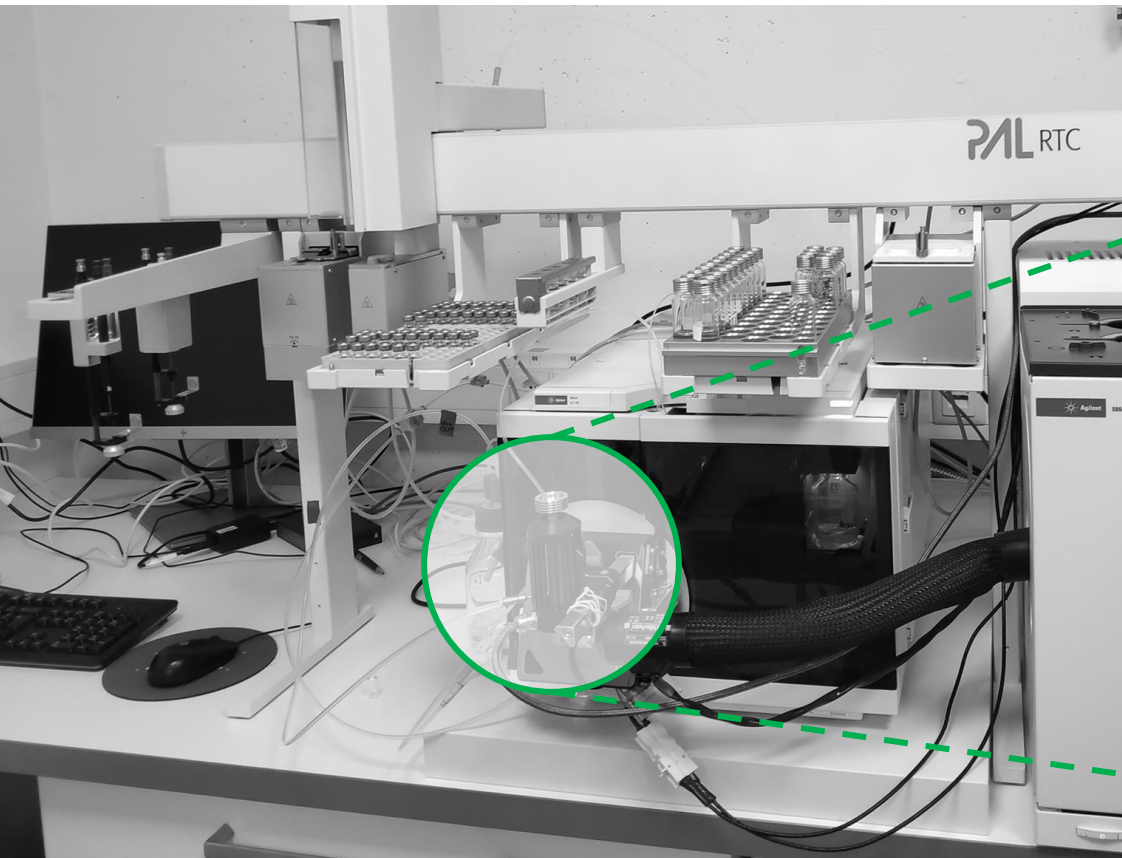
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Screening with quantification

In other cases, **screening** is not sufficient as additionally the **quantification** of specific analytes may be required:

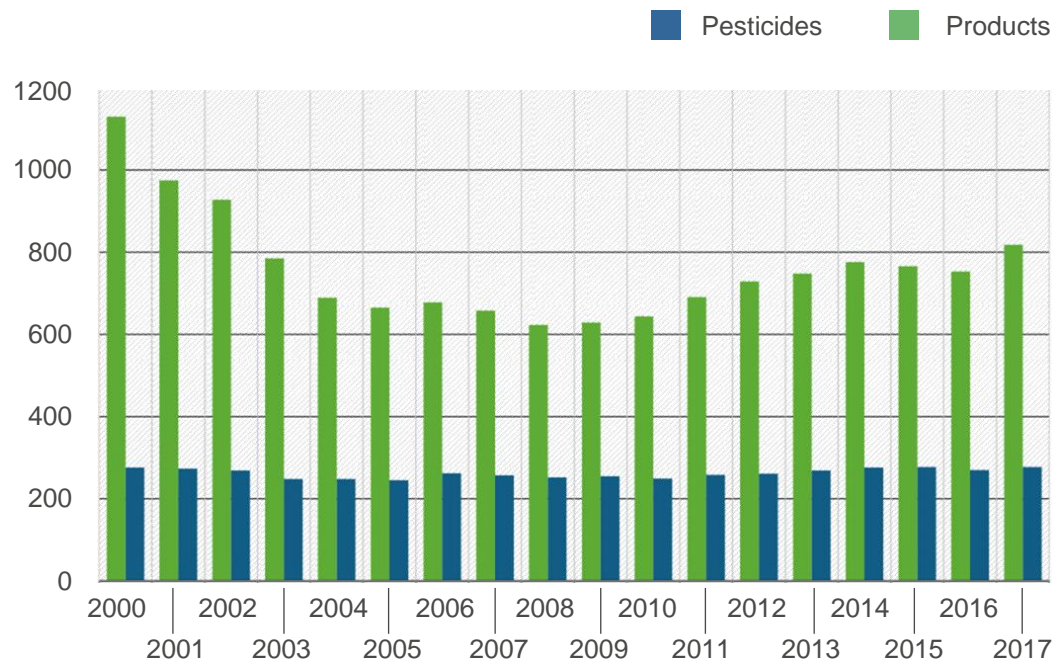
- Identifying the chemical composition of unknown samples and **determining** the **extent** of contamination in **absolute terms**

2 Via its GC-SPME-Module, SICRIT® allows for automated and quantitative direct screening experiments



2 Contaminations of food and water are a major topic in routine analytics – e.g. pesticides

Almost 300 legally authorized pesticides available



Source: Bundesamt für Verbraucherschutz und Lebensmittelsicherheit

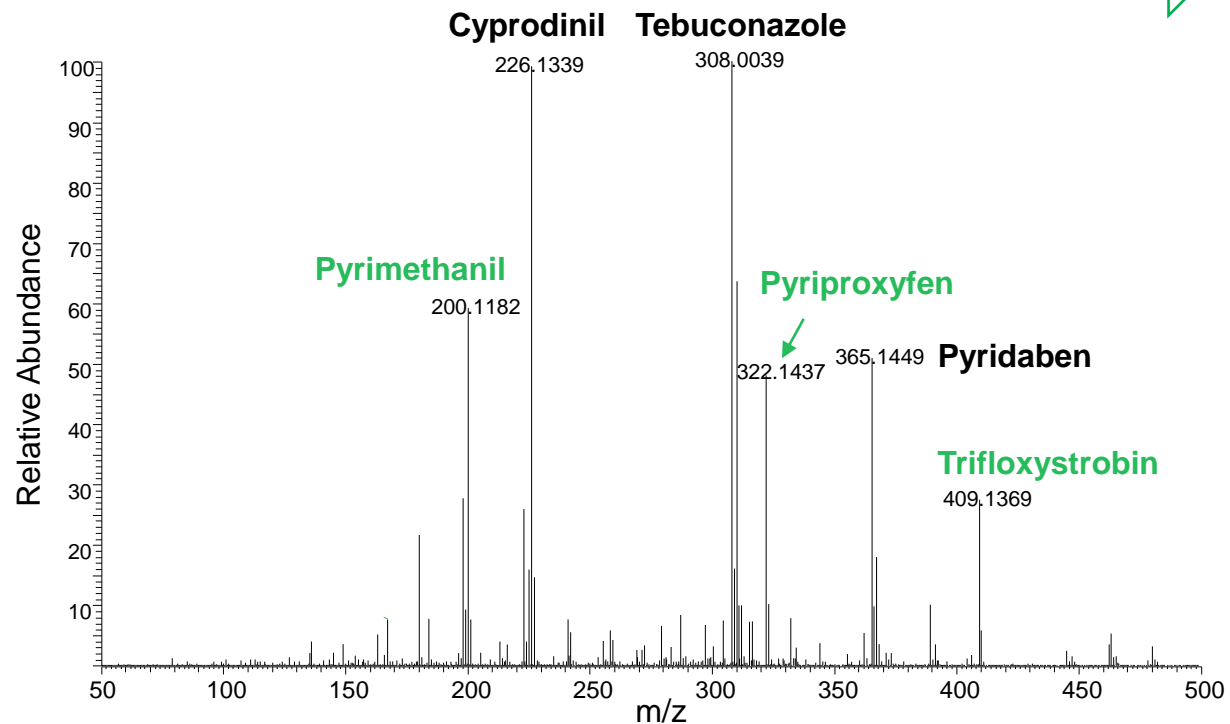
Pesticide analytics: Status quo

Pesticides are a large group of very different chemical compounds. **Analytics** are usually very **complex** as it needs to be conducted based on a **combination of GC-MS and LC-MS**:

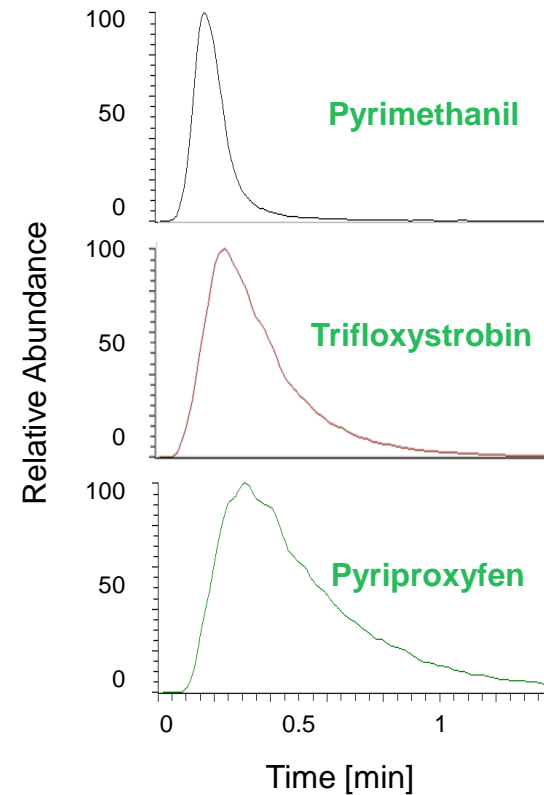
- **Tedious sample preparation** (e.g. cutting, extraction) and analyte enrichment
- Analyte **separation is obligatory**
- Very **low threshold** values especially in food and water samples

2 SICRIT[®] enables simultaneous quantification of different pesticides desorbed from a SPME fiber

Soil Sample spiked with pesticides (100 ng/mL)



SPME Desorption

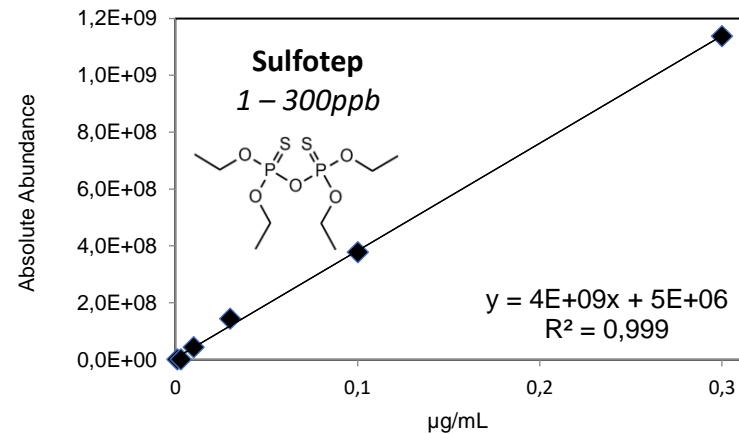
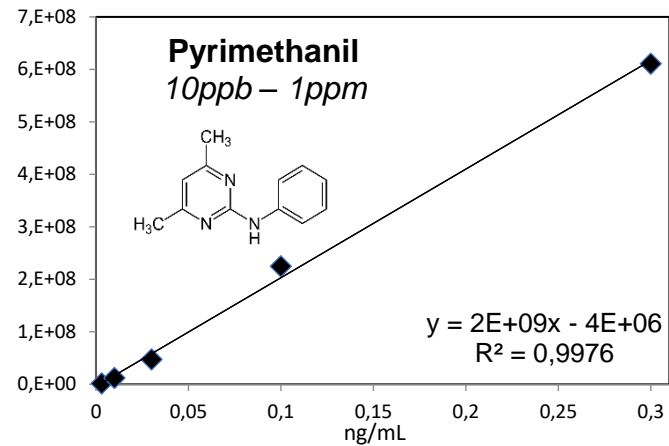
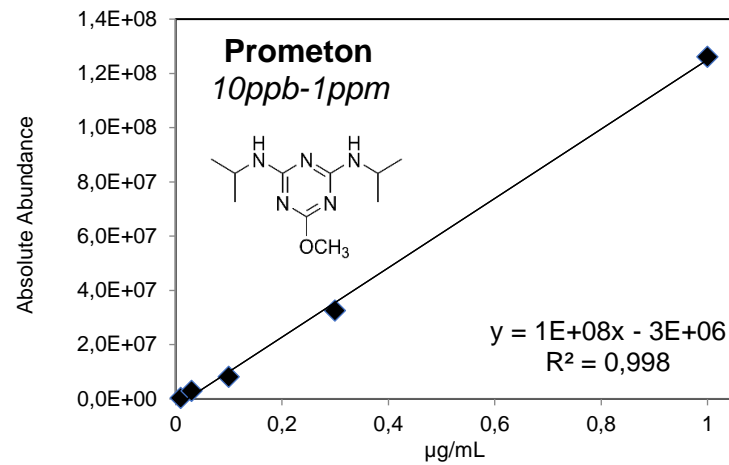


Conclusion

- Direct screening of complex matrices
- Simultaneous quantification of several pesticides
- Quantification without chromatography even on ppt level

2 SICRIT[®] delivers high reproducibility, good linear dynamic range and high sensitivity without chromatography

Calibration Curves of different analytes:

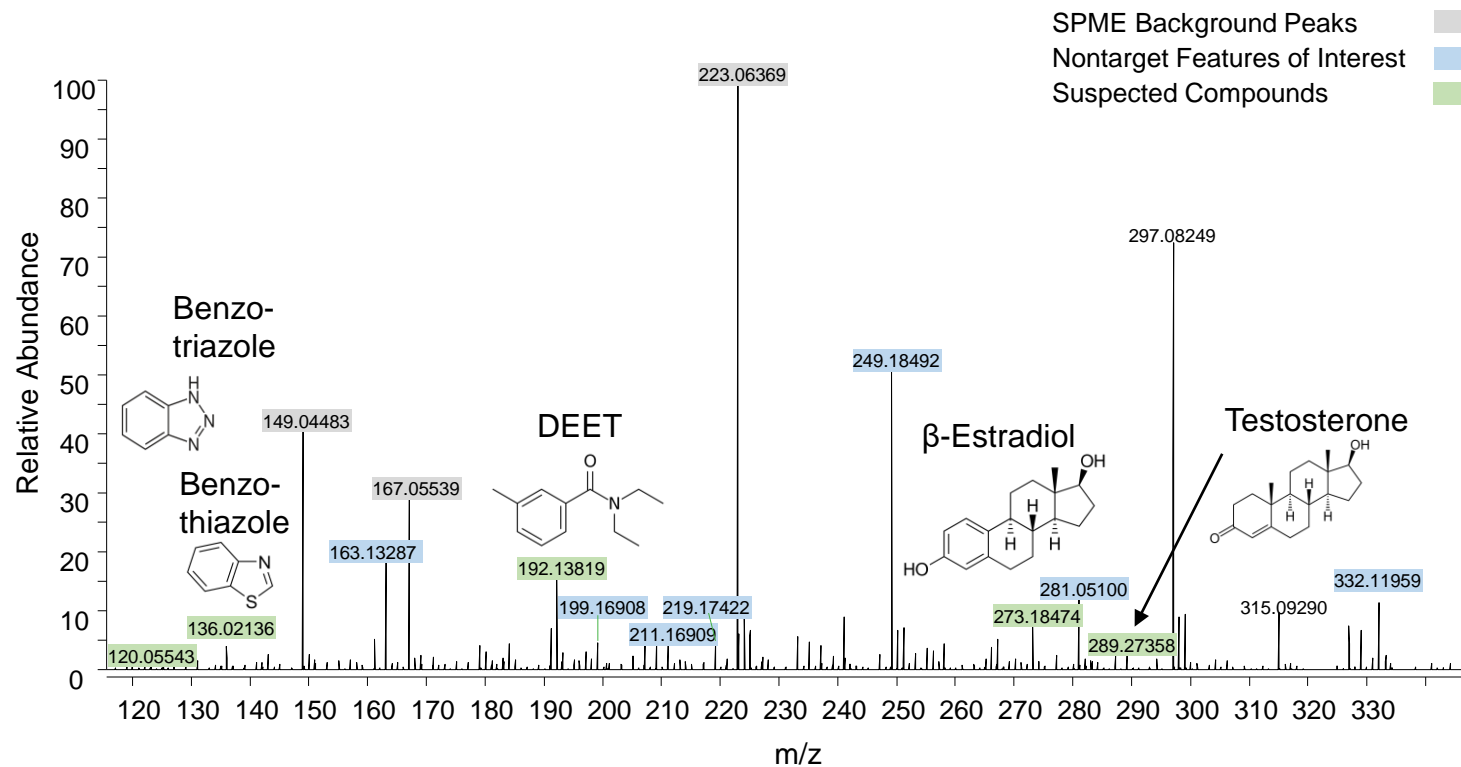


Quantification characteristics

- Linear Dynamic Range LDR > 2 orders of magnitude
- High sensitivity with LODs in the ppt range
- Good intra-day reproducibility:
 - $\leq 10\%$ for mid calibration range
 - $\leq 25\%$ for calibration extremes

2 | Also complex matrices can be analysed and quantified while additional non-target information is gained (2/2)

SPME-SICRIT-HRMS spectrum of wastewater sample



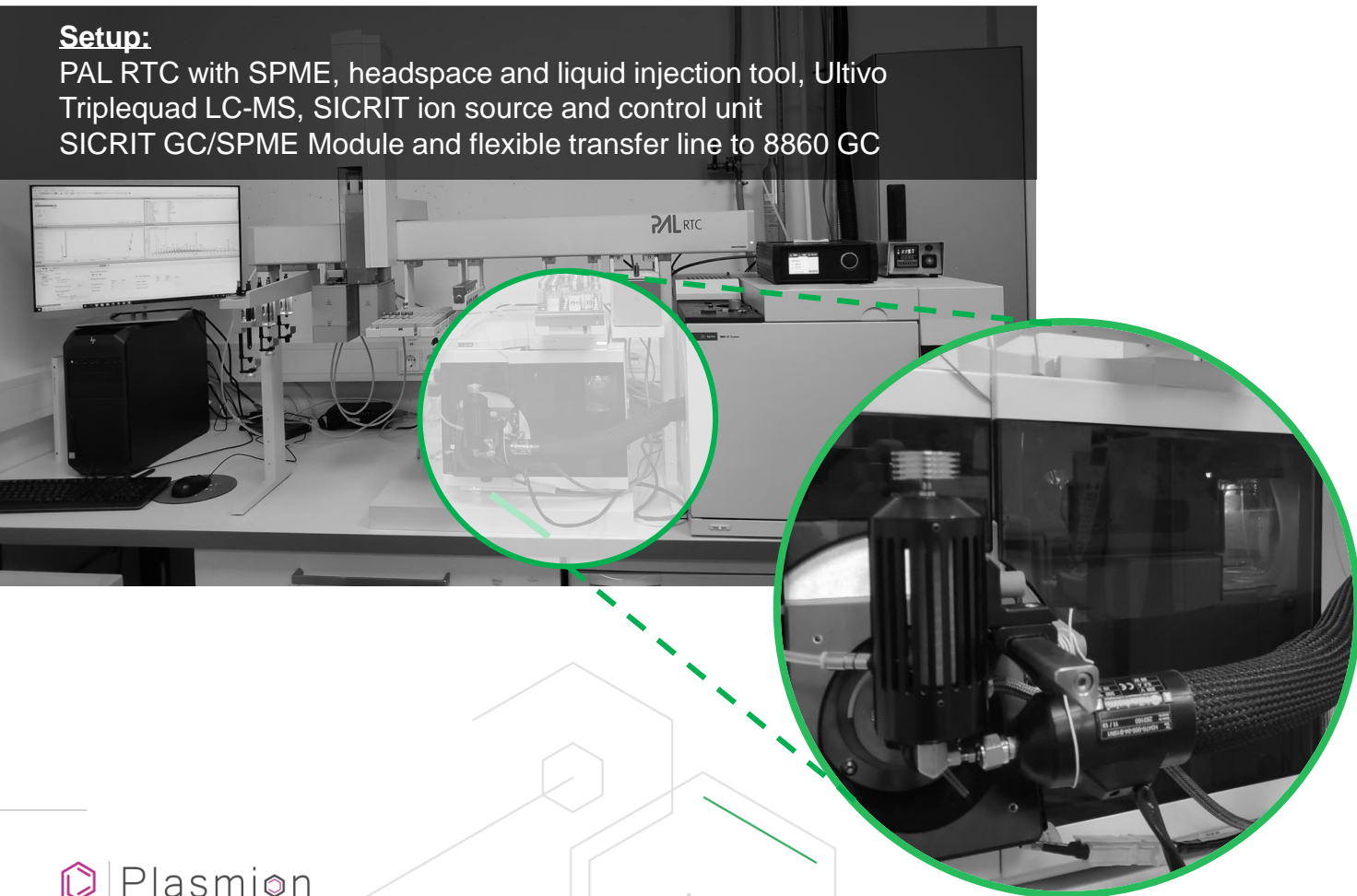
Conclusions

- **Matrix effects < 30%** for all water matrices tested (tap, ground, spring, lake, surface, wastewater)
- In addition to the **quantified compounds** (at high ppt - low ppb levels), several **unexpected compounds** were **detected** in the treated wastewater as well as the wastewater effluent mixing zone

2 SICRIT® all in one setup increases efficiency of routine analytics by combining MS screening and GC-MS

Setup:

PAL RTC with SPME, headspace and liquid injection tool, Ultivo Triplequad LC-MS, SICRIT ion source and control unit
SICRIT GC/SPME Module and flexible transfer line to 8860 GC



Background:

In routine analytics, many samples are investigated by GC-MS.

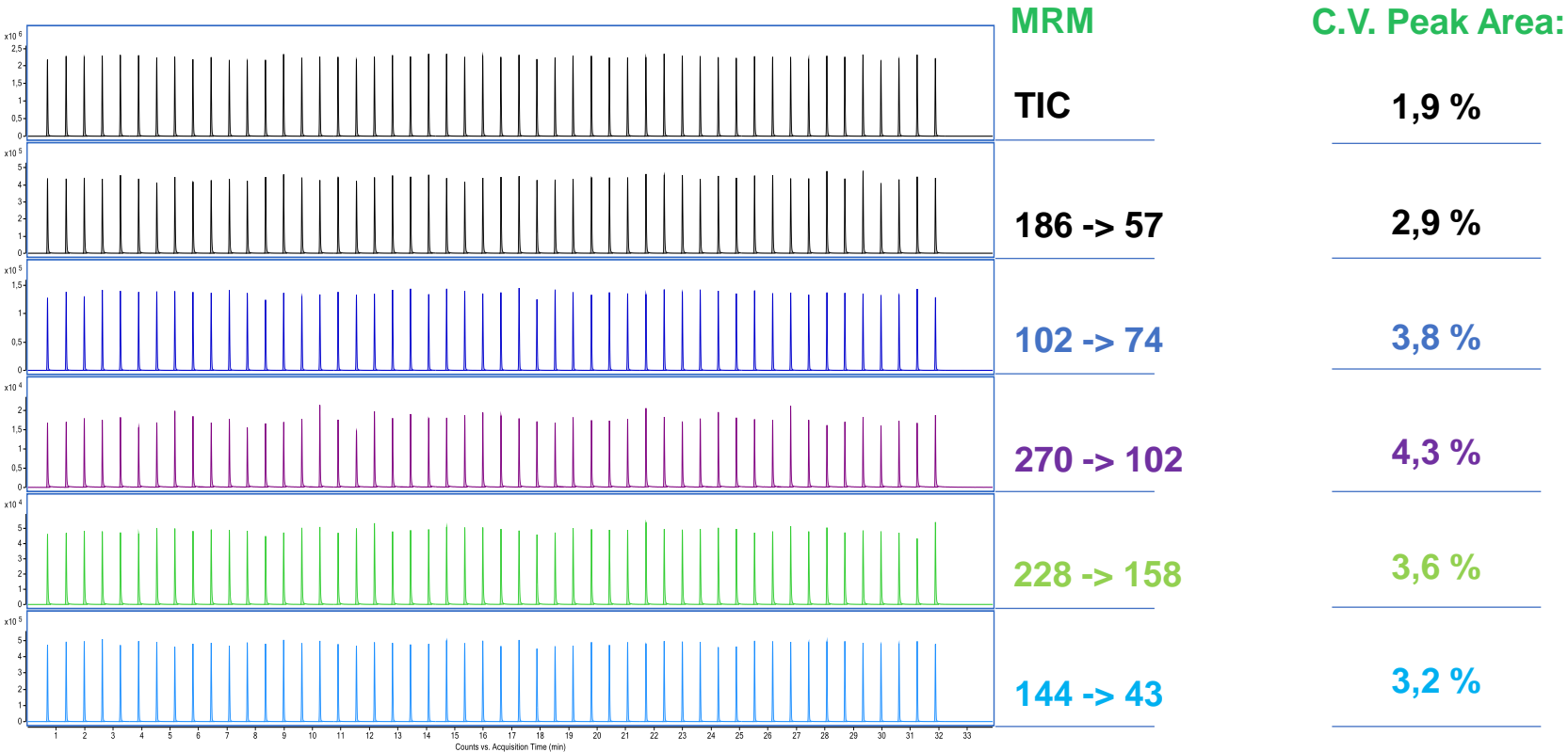
With Plasmion's new all in one set up it is possible to investigate only conspicuous samples, i.e. those screened to be positive. The combination with a PAL autosampler enables to completely automate this **2-step workflow**:

1. Direct and automated screening (infusion) of the sample to check if the sample contains a suspected compound (e.g. pesticide)
2. If the sample is positive, automated injection into the GC for a routine GC-MS run.

50 consecutive direct 1 µl injections show excellent reproducibility even without internal standard



Chromatograms



Conclusion

- Excellent reproducibility in 50 consecutive direct injections
- Less than 5% derivation of peak areas
- Super sensitive due to MRM transitions
- Quantification of several analytes at the same time

SICRIT[®] direct screening possibility provides three advantages for existing (routine) analyses



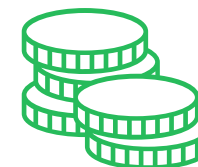
Direct screening enables fast identification and comparison of substances:

Fast & Direct Screening enables to identify or compare different substances without any sample preparation



Screening with quantification delivers reliable concentration levels:

Screening with quantification not only enables a fast identification of substances but also provides reliable information about concentration levels to compare with standards or thresholds



Automated all-in-one workflow simplifies routine analytics:

All-in-one-Workflow reduces effort and cost in routine analytics as it enables to only perform detailed GC-MS analysis for positively screened samples

Besides its universal application, SICRIT[®] screening provides advantages over other dedicated methods



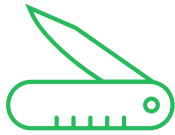
Direct Screening

GC/MS Coupling

LC/MS Coupling

SFC/MS Coupling

Laser Ablation Imaging



Compared to ASAP and DART, SICRIT[®] provides several **advantages** for direct screening applications:

- Capable to analyze solid, liquid and gaseous samples
- Provides possibility for **remote sampling** and **online monitoring**
- Enables **quantitative measurements**
- Higher **sensitivity**

✓	✓	✓	✓
✗	✗	✗	✗
✗	✗	✗	✗

Thanks for your attention!

Interested in more information?

Get in touch!



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