

A MINIATURE, DEPLOYABLE MASS SPECTROMETER FOR THE DIRECT ANALYSIS OF AROMA-RELATED VOCs IN ESSENTIAL OILS.

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INTRODUCTION & AIM



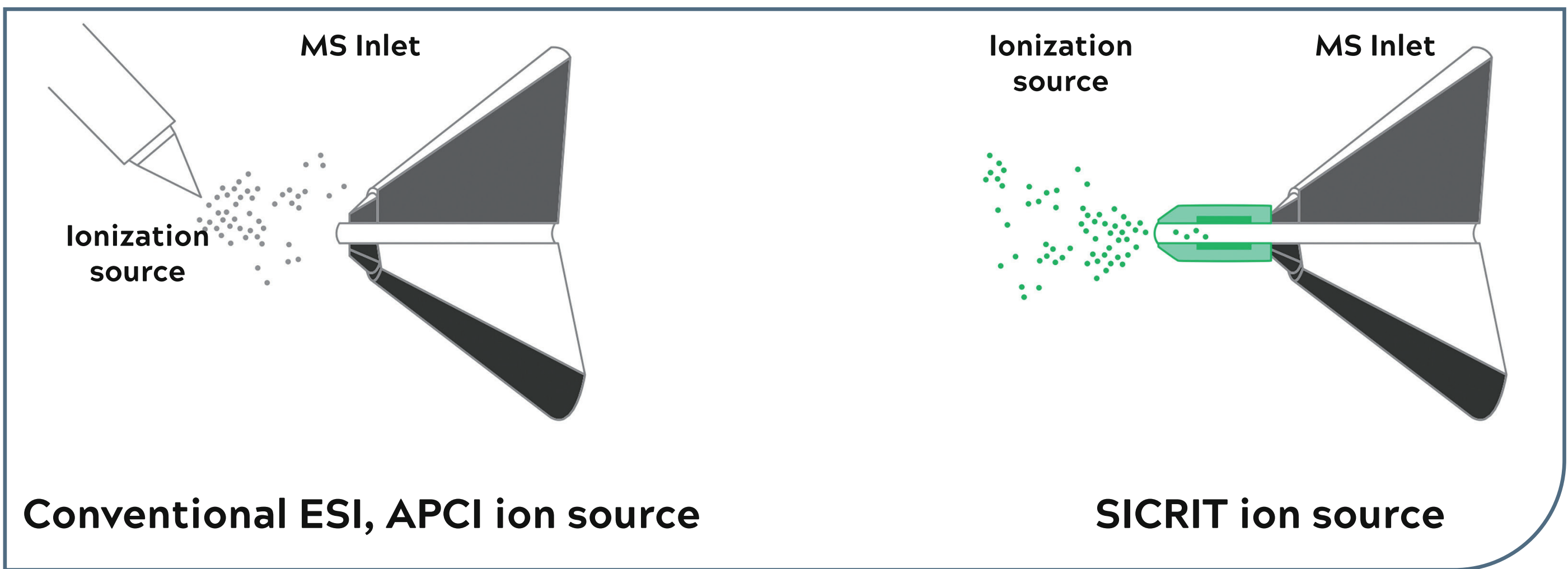
The development of portable analytical instruments, including mass spectrometers, has progressed rapidly in recent years. A new transportable instrument is now available that provides MS and MS/MS data quality comparable to that of benchtop systems. The aim of this study was to develop a real-time approach for the characterization of essential oils using this portable platform. Ideally, this methodology enables on-site analysis directly at the production facility, providing an ultra-fast assessment of product quality and authenticity.

MINIATURE MS/MS



An innovative field-deployable MS (MTE30, MassTech Inc., Columbia) equipped with an atmospheric-pressure interface has been coupled with a ring-shaped cold plasma ion source (SICRIT, Plasmion, Augsburg). The instrument¹ is fully integrated into a single chassis, requires no external pumps or gases, weighs approximately 17 kg, and provides better-than-unit mass resolution over a 2000 Da range. MS/MS acquisitions are also possible, enhancing instrumental specificity for complex samples.

DIELECTRIC BARRIER DISCHARGE IONIZATION (DBDI/MS)



With DBD² ionizations (SICRIT ion source, Plasmion GmbH), the inlet of the MS is extended and all molecules are drawn into the system are ionized by means of a cold plasma. Resulting in a high ionization efficiency and very high sensitivity for real-time analysis^{3,4}.

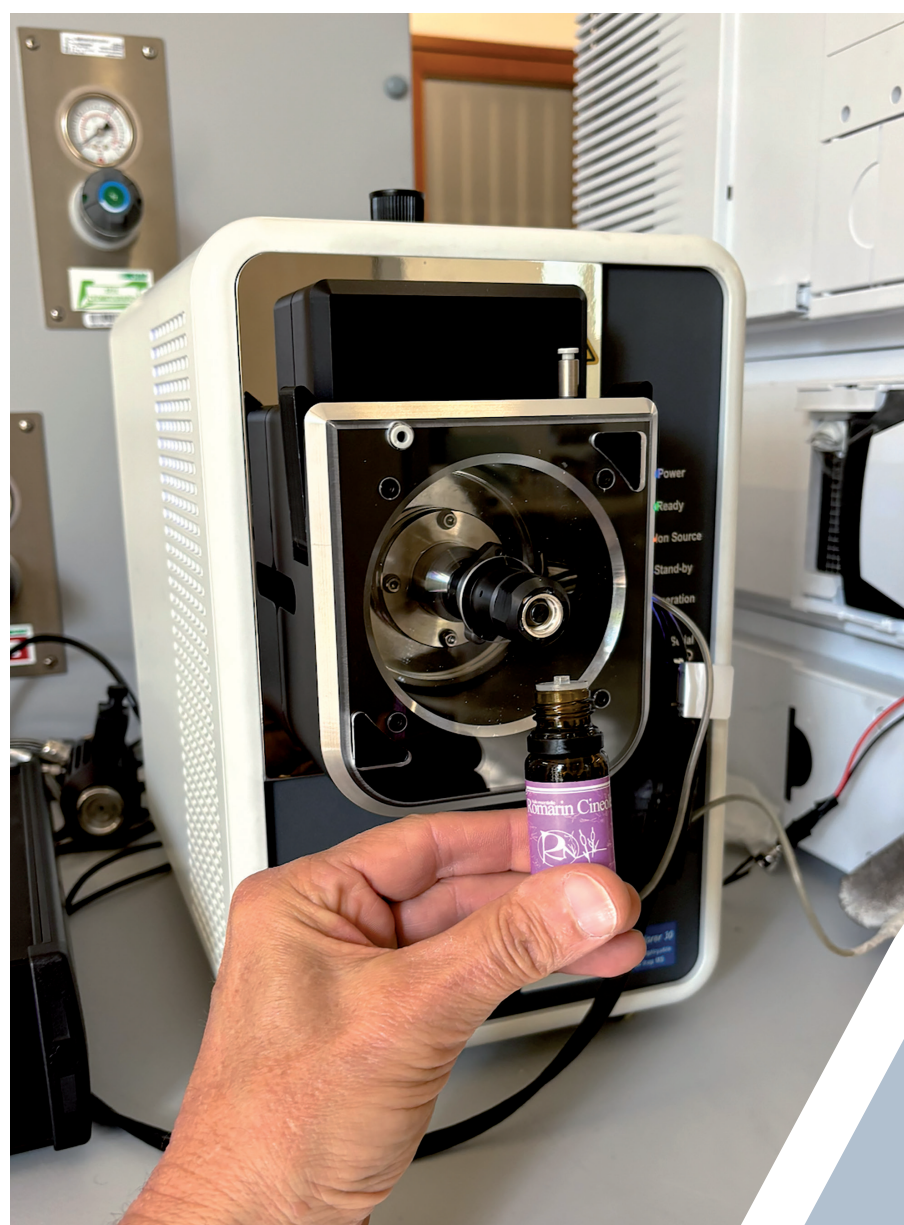


Main SICRIT ion source advantages are:

- Enhanced range of polarity
- No or minimized fragmentation
- Versatility: direct MS, GC/MS, LC/MS, SFC/MS, MS imaging
- Installation is quick and easy. Plug-and-play
- Interfaces available for most MS manufacturers.

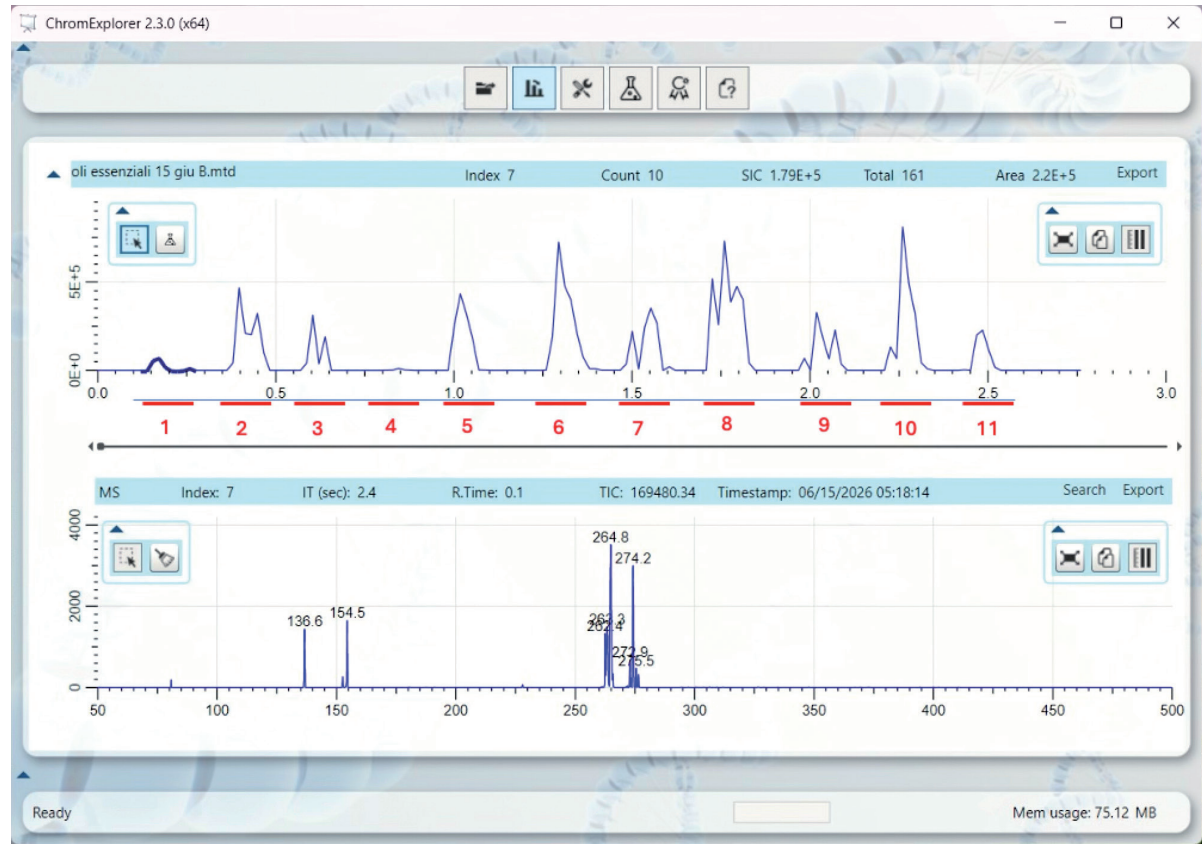
SAMPLE PREPARATION

No sample preparation was required. The essential oils were analyzed directly by exposing the sampling cone of the mass spectrometer to their headspace vapors through the SICRIT ion source.

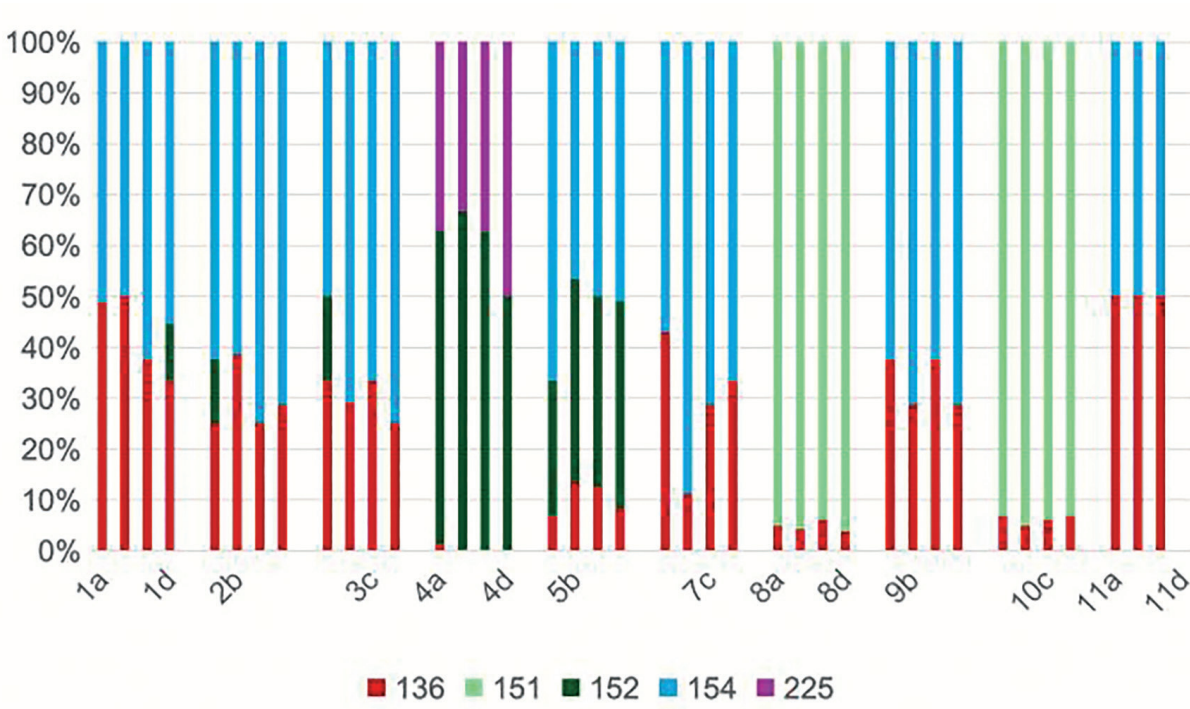


RESULTS

Fast sample classification: 5 seconds/sample. Replicate 1/4



Ten samples two aromas different producers Essential oil



DIRECT HEAD-SPACE ANALYSIS

Classification	
7	Rosmarino a Cineole
8	Rosmarino terapeutico canfora
9	Bio Rosmarino
10	Rosmarino canfora
11	Romarin natuell

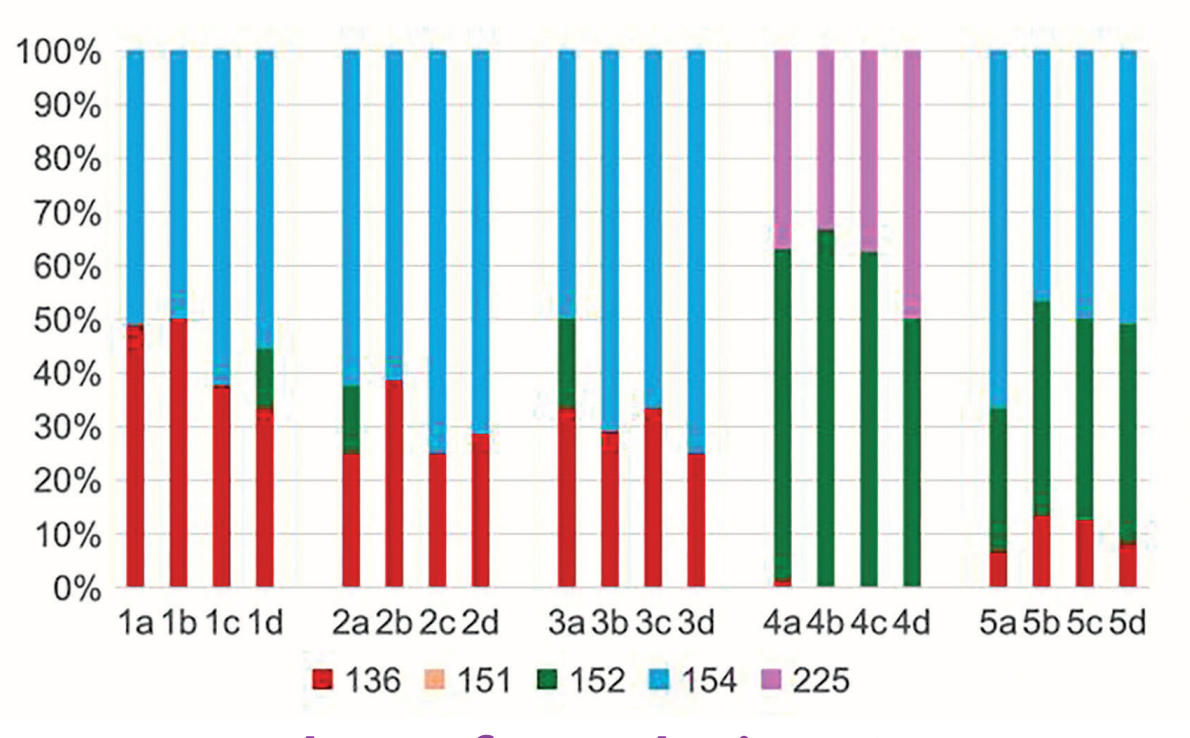
DIRECT HEAD-SPACE ANALYSIS

Classification	
1	Lavande Aspic A
2	Lavande Aspic B
3	Lavanda Spike
4	Fine Lavander
5	Spike Lavander

OUTPUT Rosemary

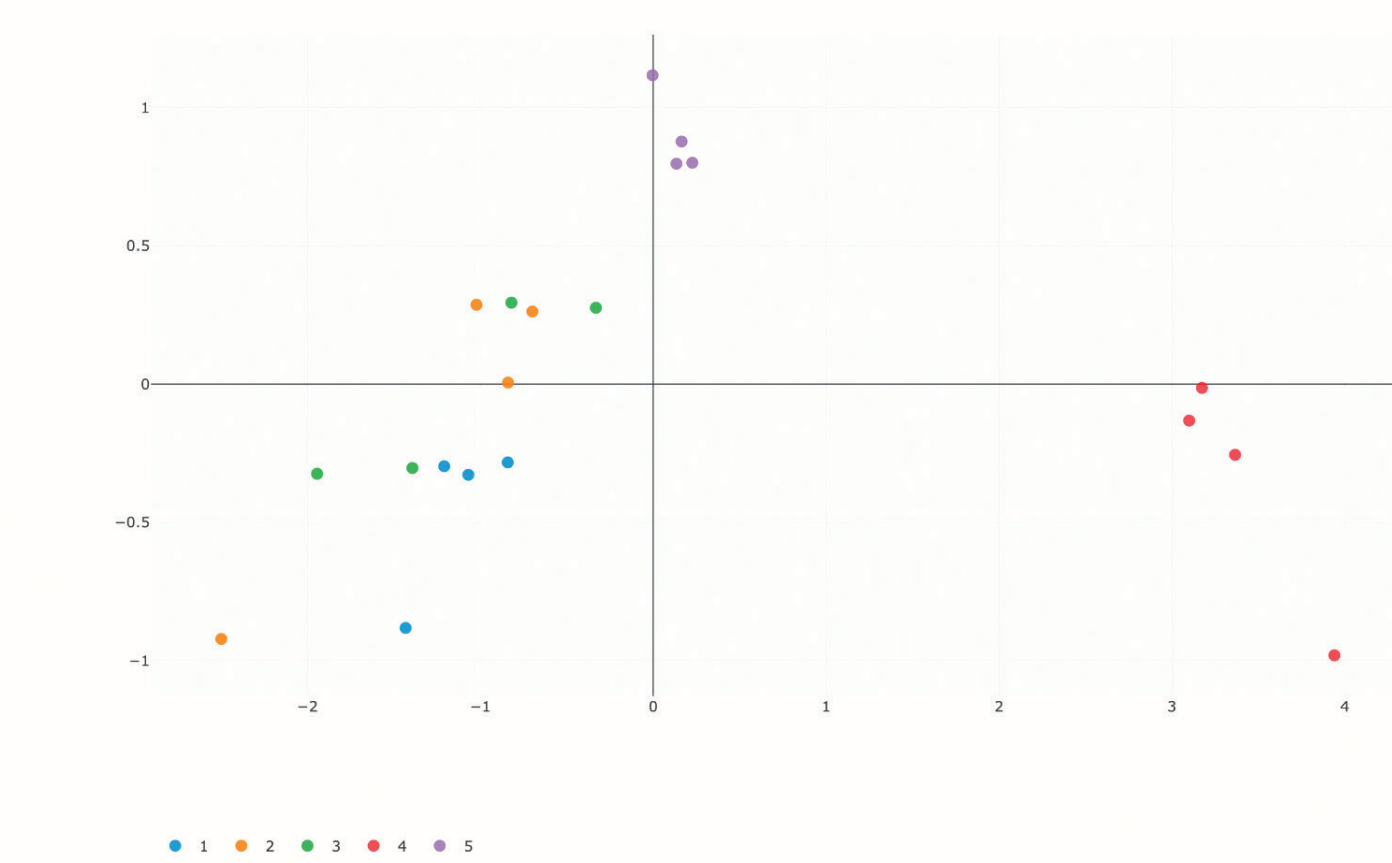


OUTPUT Lavender



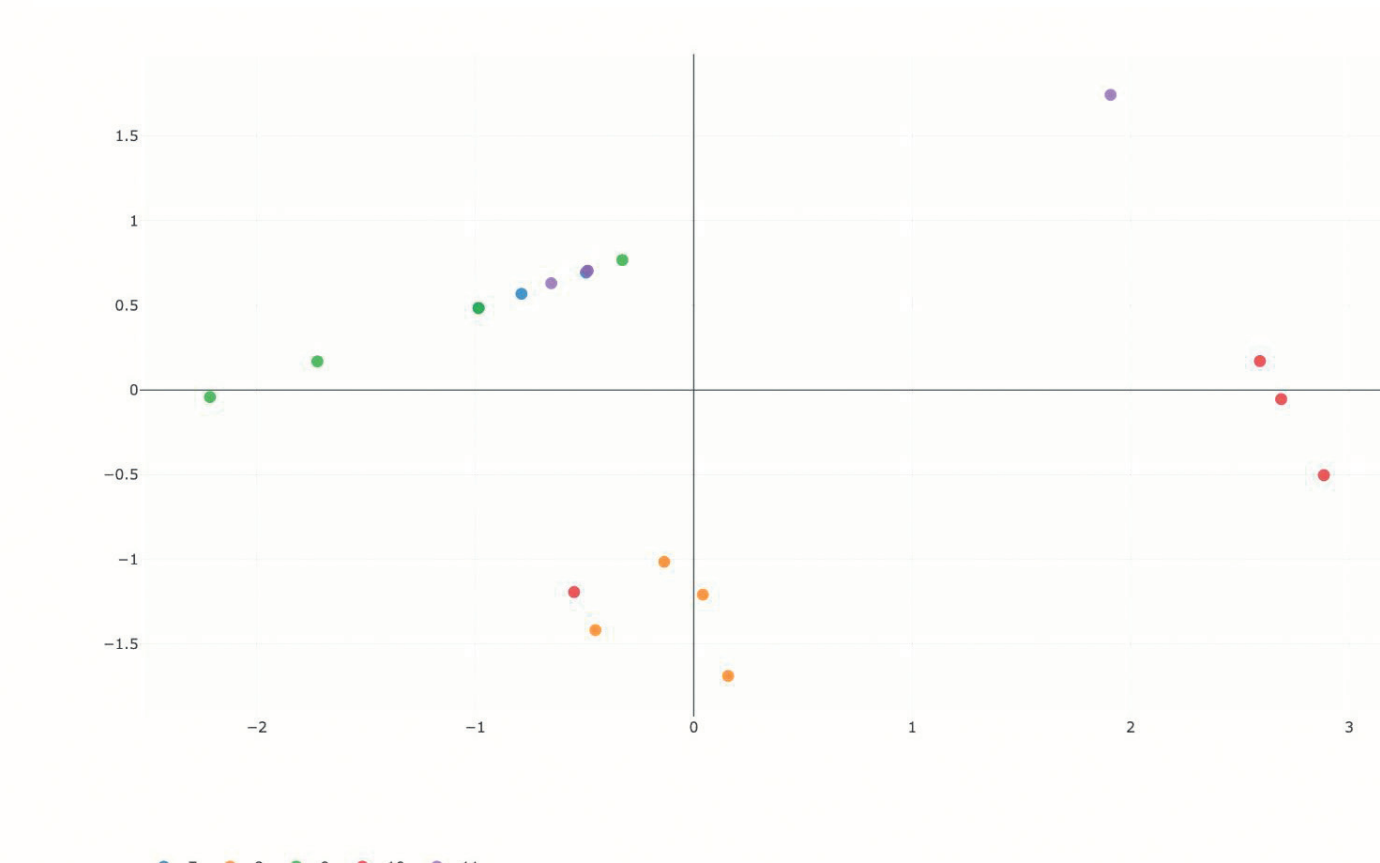
Results: PCA analysis

2D Score Plot (PC1 vs PC2)



Rosemary samples

2D Score Plot (PC1 vs PC2)



Lavender samples

CONCLUSIONS

■ Miniature, Transportable, Instrumentation

A mature technology that is becoming indispensable for specialized analyses.

■ Direct Analysis

Fast, sample prep-free, accurate. Easy installation on full size as well as on miniature MS instrumentation.

■ Classification by Direct Analysis

Essential oils from different manufacturers can differ, although some samples appear to have similar formulations.

REFERENCES

[1] Development and Characterization of a Field-Deployable Ion-Trap Mass Spectrometer with an Atmospheric Pressure Interface. Anal. Chem. 2012, 84, 22, 10105-10112.
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[3] Real-time breath analysis with active capillary plasma ionization-ambient mass spectrometry. Journal of Breath: J. Breath Res. 8 (2014) 027102.
[4] Real-time monitoring of tea volatiles using soft ionization by chemical reaction in transfer with an on-line sampling interface. Green Analytical Chemistry 2025, 100290, Volume 14.