APPLICATION NOTE 65914

# Intelligent omics workflow using an Orbitrap Exploris GC 240 mass spectrometer for food characterization

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## Goal

The aim of this application note is to demonstrate the performance of the Thermo Scientific™ Orbitrap Exploris™ GC 240 coupled to SPME Arrow technology for the assessment of the aroma profile in *Origanum vulgare* samples grown in different geographical areas.

## Introduction

*Origanum vulgare* is widely used as an ingredient and flavoring for culinary purposes because of its organoleptic properties and enjoyable taste.[1]

Oregano is a complex matrix with an extremely variable composition of phytosterols, pigments, and essential oils. The differences in the amounts of its major constituents can be used to discriminate between individual plants. For example, the monoterpene content is strongly affected by the climatic conditions playing an important role in up/downregulating the cymyl-, sabinyl-, and linalool/linalyl acetate pathways.[2] Plants originating from the Mediterranean climate usually exhibit active cymyl- and/or linalool pathways, with the first being characterized by a higher content of carvacrol, thymol, and their biosynthetic precursors (*γ*-terpinene and *p*-cymene) and the second one characterized by higher concentration of linalool and linalyl acetate. Plants originating from continental climate are usually poorer in monoterpenes, showing a higher content of sesquiterpenes (mainly sabinene and *trans/cis*–sabinene hydrate and their acetates) generated by the sabinyl-pathway.[2]

Flavor analysis presents some challenges as the number of compounds that must be extracted from the matrix and identified is significant. Moreover, these chemicals usually have different chemical properties (structure, reactivity, polarity, boiling point). Aroma compounds can be present at very low concentrations; therefore, their extraction, identification, and quantitation become critical to obtain reliable results. Oregano aroma compounds can be extracted using different techniques such as distillation, Soxhlet extraction, static-headspace sampling (SHS), and purge and trap (P&T), although they have some limitations. Monoterpenes can undergo chemical changes under the conditions applied for distillation, while volatile compounds can be lost with solvent extraction. Static headspace and purge and trap can result in low sensitivity and risk of cross-contamination. Headspace solid phase micro-extraction (HS-SPME) has become common in aroma analysis as it is rapid, simple, and allows for the extraction of volatile and semi-volatile compounds with minimal sample preparation, which is a critical point in non-targeted analysis since every manipulation could alter the sample composition.[3]

Flavor analysis can be carried out using either liquid or gas chromatography coupled to mass spectrometry (LC or GC–MS) or high resolution accurate mass mass spectrometry (LC or GC-HRMS) and the use of effective software tools for data reprocessing and statistical analysis. The high resolution GC approach with the Orbitrap system offers the advantage of full-scan data acquisition combined with high sensitivity, high resolving power (up to 240,000 FWHM at *m/z* 200), and accurate mass (<1 ppm), allowing for targeted, non-targeted, and retrospective data analysis.[3]

In this study, the Orbitrap Exploris GC 240 system coupled to SPME Arrow technology was used to assess the aroma profile of several *Origanum vulgare* samples grown in different geographical areas with either Mediterranean or continental climate. Data was acquired in full-scan (FS) electron ionization (EI) and positive chemical ionization (PCI) modes, and reprocessed using the streamlined workflows integrated in the Thermo Scientific™ Compound Discoverer™ 3.2 software platform.

## Experimental

In all experiments, an Orbitrap Exploris GC 240 system with a Thermo Scientific™ Instant Connect split/splitless SSL (equipped with SPME Arrow liner 1.7 mm ID (P/N 453A0415)) was coupled to a Thermo Scientific™ TriPlus™ RSH autosampler with SPME Arrow configuration. In place of the standard SPME Arrow Conditioning Station, a second IC-SSL injector (equipped with SPME Arrow liner 1.7 mm ID (P/N 453A0415)) was used for fiber conditioning. Chromatographic separation was achieved using a Thermo Scientific™ TraceGOLD™ TG-1MS capillary column, 30 m × 0.32 mm × 1.0 µm (P/N 26099-2970). Additional HS-SPME Arrow and Orbitrap Exploris GC 240 system parameters are detailed in Tables 1a and 1b, respectively. The triple coating phase of the DVB/CWR/PDMS fiber (P/N 36SA11T3) allowed for effective extraction of monoterpenes, cyclic and acyclic terpenes, sesquisterpenes, and bornane compounds.

**Table 1a. TriPlus RSH-SPME Arrow experimental parameters used for the assessment of the volatile fraction of oregano**

| TriPlus RSH – HS - SPME Arrow parameters | |
|---|---|
| Fiber | SPME Arrow DVB/CWR/PDMS (P/N 36SA11T3) |
| Coating phase thickness (µm) | 110 |
| Coating phase length (mm) | 20 |
| Incubation temperature (°C) | 60 |
| Incubation time (min) | 15 |
| Incubation speed (rpm) | 500 |
| Extraction temperature (°C) | 60 |
| Extraction time (min) | 15 |
| Stirring speed (rpm) | 1500 |
| Fiber depth in vial (mm) | 25 |
| Fiber depth in injector (mm) | 70 |
| Desorption time (min) | 2 |
| Analysis time (min) | 40 |
| **Fiber conditioning** | |
| Inlet temperature (°C) | 270 |
| Liner | SPME Arrow liner 1.7 mm I.D. (P/N 453A0415) |
| Inlet module and mode | SSL, splitless |
| Fiber pre-conditioning time (min) | 0 |
| Fiber post-conditioning time (min) | 15 |
| Septum purge flow (mL/min) | 5, constant |
| Carrier gas (mL/min) | He, 6.0 |
| Fiber depth in injector (mm) | 70 |

**Table 1b. Trace 1310 GC and Orbitrap Exploris GC 240 mass spectrometer experimental parameters used for the assessment of the volatile fraction of oregano**

| Trace 1310 GC parameters | |
|---|---|
| Inlet (°C) | 220 |
| Liner | Arrow liner 1.7 mm I.D. (P/N 453A0415) |
| Inlet module and mode | SSL, split |
| Split ratio | 30:1 |
| Septum purge flow (mL/min), mode | 5, constant |
| Carrier gas (mL/min) | He, 1.8 |
| **Oven temperature program** | |
| Temperature (°C) | 40 |
| Hold time (min) | 2 |
| Rate (°C/min) | 10 |
| Temperature 2 (°C) | 150 |
| Rate (°C/min) | 5 |
| Temperature 3 (°C) | 260 |
| Rate (°C/min) | 25 |
| Temperature 4 (°C) | 300 |
| Hold time (min) | 3 |
| **Column** | |
| TraceGOLD TG-1MS | 30 m, 0.32 µm, 1.0 mm (P/N 26099-2970) |
| **Vials and caps** | |
| Vials | 10 mL crimp top HS vials (P/N 10-CV) |
| Caps | 20 mm magnetic crimp caps (P/N 20-MCBC-ST3) |
| **Orbitrap Exploris GC 240 mass spectrometer parameters** | |
| **Parameters for EI** | |
| Transfer line temperature (°C): | 280 |
| Ionization type: | EI |
| Ion source temperature (°C): | 280 |
| Electron energy (eV): | 70 |
| Aquisition mode: | Full Scan |
| Mass range (Da): | 40–450 |
| Resolving power (FWHM): | 60,000 @ *m/z* 200 |
| Lockmass, column bleed: | 207.03235 |
| **Parameters for PCI** | |
| Transfer line temperature (°C): | 280 |
| Ionization type: | CI |
| Ionization gas: | Methane |
| Ionization gas flow (mL/min): | 1.3 |
| Ion source temperature (°C): | 190 |
| Electron energy (eV): | 90 |
| Aquisition mode: | Full Scan |
| Mass range (Da): | 80–450 |
| Max resolving power (FWHM): | 120,000 @ *m/z* 200 |

### Data acquisition, processing, and reporting

Data were acquired using Thermo Scientific™ Chromeleon™ 7.3 CDS software and imported in Compound Discoverer 3.2 software for chemometric assessment. Chromeleon CDS integrates instrument control, method development functionality, and quantitation-focused workflows in compliance with Title 21 of the Code of Federal Regulations. Compound Discoverer 3.2 software was used to reprocess EI data (spectral deconvolution, compound identification, and multivariate statistical analysis) as well as CI data (elemental composition of the molecular ions and presence of specific adducts confirmation).

### Sample preparation

Three commercially available *O. vulgare* samples were purchased at different retailers. Each oregano jar was well mixed to homogenize the matrix. Herb samples were prepared in triplicate by weighing (150 mg) and transferring into 10 mL crimp top headspace vials (vials P/N 10-CV, caps P/N 20-MCBC-ST3) for analysis. A blend was obtained by pooling together the oregano samples and was used for confirmatory purposes. To reduce the bias in the results, the sample vials were analyzed in a randomized order. A retention index (RI) mix (Sigma-Aldrich, C7-C30 saturated alkanes, P/N 49451-U) was injected at the beginning of the sequence and used to derive the RI of chemical components putatively identified by the NIST™ Mass Spectral Library (NIST20) and the Thermo Scientific™ Orbitrap™ GC-MS HRAM Metabolomics Library (P/N 1R120400-0080) following spectral deconvolution.

## Results and discussion

### Workflows to assess the volatile profile in oregano samples

Full scan EI and CI data were processed using Compound Discoverer 3.2 software for chemometric assessment and putative identification of peaks as reported in Figure 1. Multivariate statistical analysis (principal component analysis, PCA and volcano plot, v-plot) was used to select the significant features, defined by their *m/z* and retention time, contributing to the group differences. Chromatographic peaks were then deconvoluted, aligned, filtered, and putatively identified using mass spectral library match (NIST20 nominal mass library and Orbitrap GC-MS HRAM Metabolomics Library). The PCI workflow in Compound Discoverer software enabled confirmation of the presence of the molecular ion and the adducts and proposal of a chemical formula. These streamlined workflows allowed for a comprehensive characterization of the aroma components in oregano samples.

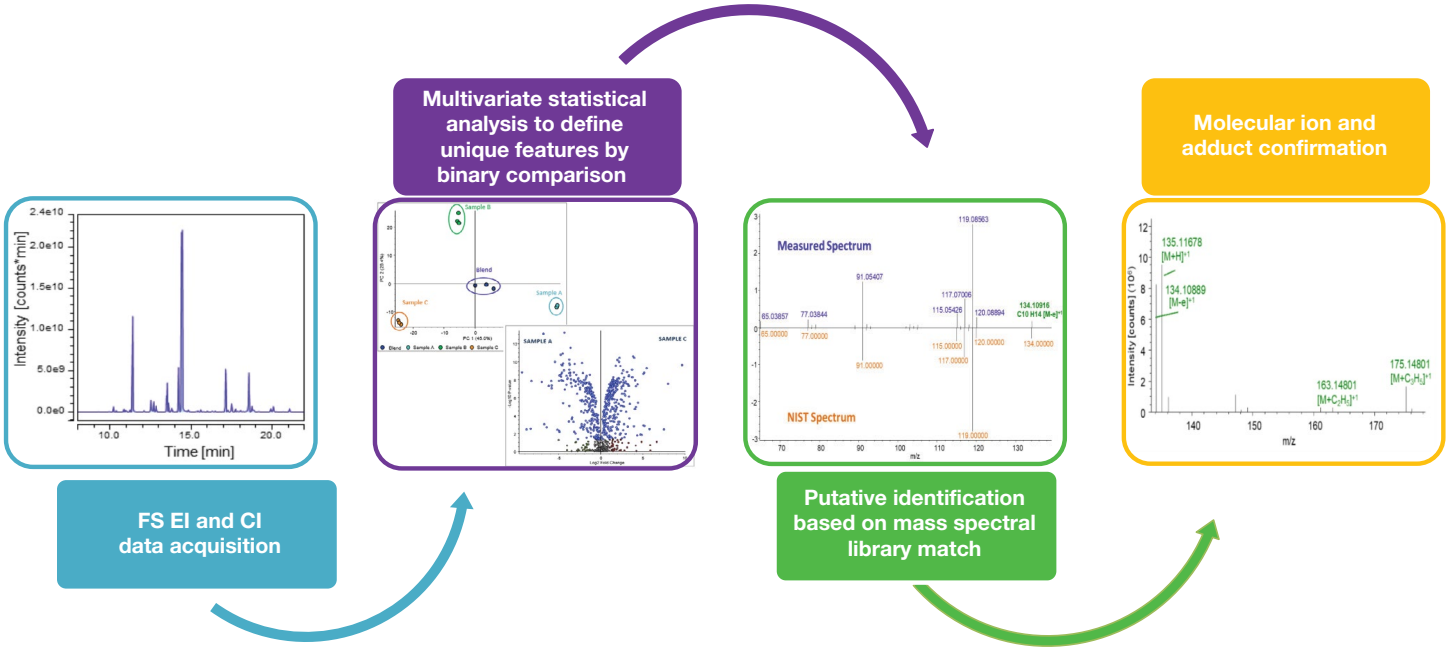



**Figure 1. Workflow used to assess the volatile profile of the oregano samples.** FS data was acquired in EI and PCI modes: multivariate statistical analysis was performed to identify unique features contributing to the group differences in EI data; peak putative identification was made using mass spectral library match (NIST20 and Orbitrap GC-MS HRAM Metabolomics Library); compound identification was confirmed using soft ionization PCI data and the presence of quasimolecular and/or adduct ions.

## Multivariate statistical analysis: PCA and V-Plot

Full scan EI data were imported in Compound Discoverer software and a multivariate statistical analysis step was carried out to assess the sample differences and to isolate the main features responsible for such variances. PCA is a well-known statistical approach that highlights variation between sample groups and allows visualization of strong patterns in complex datasets. By employing PCA analysis in Compound Discoverer software, significant differences were observed between the volatile profiles of the analyzed oregano samples. The generated PCA plot is reported in Figure 2, highlighting a clear separation between the oregano samples with the blend (pooled samples) centered in-between the groups. To isolate the chemical components responsible for these variances, differential analyses were carried out using the volcano-plots, useful to quickly identify changes in large data sets composed of replicate data. A V-plot obtained by comparing sample A and sample C is shown as an example in Figure 3.

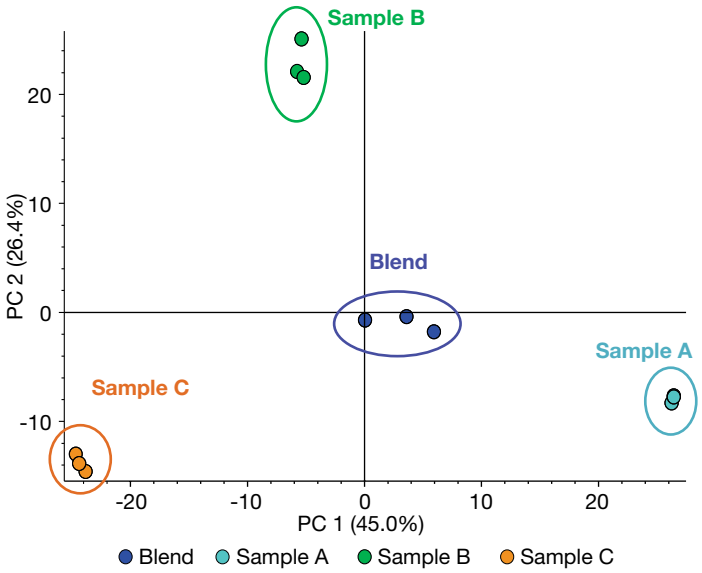



**Figure 2. Centered PCA score plot obtained for oregano samples.** The PCA plot shows a complete separation between the sample classes with the blend (pooled) samples in the clustered in the center of the plot.

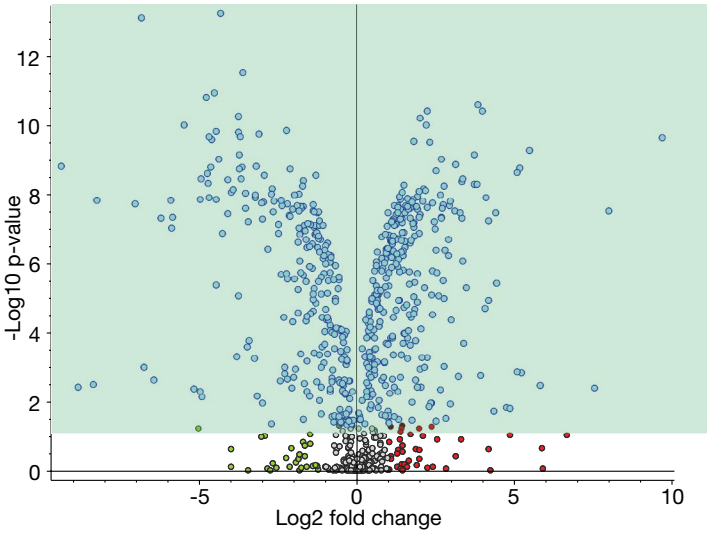



**Figure 3. Volcano-plot scatterplot showing the statistical significance (p-value) versus magnitude of change (fold change) when comparing sample A and C.** Significant chemical components that are responsible for sample diversity between two groups are selected (as light blue dots).

## Compound identification based on NIST20 and Orbitrap GC-MS HRAM Metabolomics Library match

Compound Discoverer 3.2 platform includes a streamlined workflow for GC EI data, which allows for extraction, deconvolution, and putative identification of the unknowns based on mass spectral library matching. The software first performed untargeted peak detection within 5 ppm extraction windows. Accurate mass chromatographic deconvolution was then performed by grouping together all extracted ion peaks above a customizable signal to noise (S/N) threshold that maximize at the same retention time. The deconvoluted spectra were then searched against the NIST20 nominal mass spectral library and Orbitrap GC-MS HRAM Metabolomics Library and the hits were scored based on the total score derived from a combination of library search index (SI), high resolution filtering (HRF) value and presence/absence of the molecular ions as well as elemental percentage match. The use of a retention index acquired under the same conditions used for sample analysis helped to boost the confidence in compound identification. An example of this workflow is reported in Figure 4 with the Compound Discoverer 3.2 browser showing the overlaid extracted ion chromatograms (XIC) of the peak eluting at 10.21 min (*m/z* 119.08563), the result table with the top hit for peak deconvolution and library search (NIST20 and Orbitrap GC-MS HRAM Metabolomics Library), and the EI spectrum – measured versus the NIST20 library. According to the NIST20 library, the peak was putatively identified as *p*-cymene with a total score of 95.2, SI = 796, and HRF = 98.1.

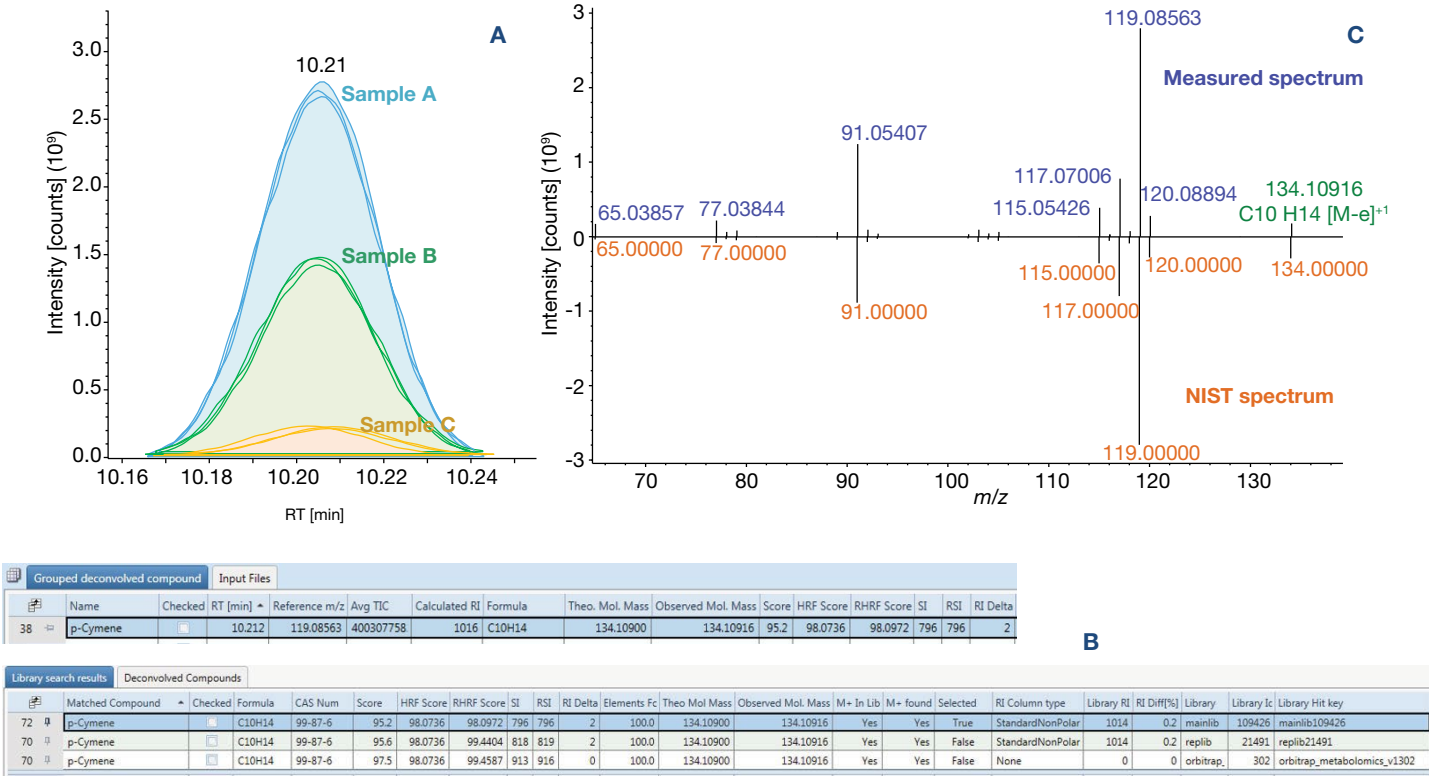



**Figure 4. Compound Discoverer software showing peak deconvolution results for the compound eluting at RT = 10.21 min and putatively identified as *p*-cymene (*m/z* 119.08563).** XIC for *p*-cymene (A); result table with deconvoluted compound and library search results for NIST20 and Orbitrap GC-MS HRAM Metabolomics Library (B); EI spectrum of *p*-cymene – measured versus NIST20 library (C).

The putative identification was supported by the Orbitrap GC-MS HRAM Metabolomics Library match with a total score of 97.5, SI = 913, and HRF = 99.5. This approach allowed putative identification of most of the detected peaks; however, for some compounds the EI spectral library match resulted inconclusive. In this case, PCI data and accurate mass become essential to discriminate the chemical formula and provide confidence in identification.

### Volatile composition of *Origanum vulgare* samples of various geographical origin

The differences in the composition of the aroma profile allowed for the discrimination between samples even with a limited data set as reported in Figure 2. Sample A showed a higher content of cymyl-type compounds such as *p*-cymene (4-fold change), *γ*-terpinene (2-fold change), and thymol (3-fold change). Sample B resulted to be poor in cymyl-type compounds but richer in acyclic compounds such as β-ocimene (4-fold change) with a higher amount of sesquiterpenes such as germacrene D (2-fold change). Sample C resulted to be richer in β-ocimene and sequiterpenes such as germacrene D and β-caryophyllene. The differences in the chemotypes can be representative of the different climate where *O. vulgare* varieties were grown with the predominance of phenolic monoterpenes in plants grown in the Mediterranean area and sesquiterpenes predominant in continental regions, although as reported in literature, oregano characterization is difficult due to the huge diversity in the aroma composition of the existing oregano populations.[2]

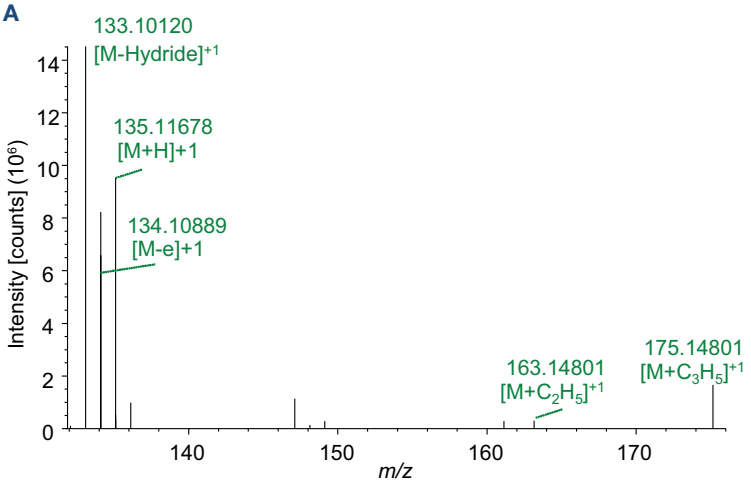
### Molecular ion and adduct confirmation using PCI

Further confirmation in the identification of compounds was achieved by assessing the PCI spectra to identify the elemental composition of the parent ion by looking at common adducts. In PCI experiments using methane as the reagent gas, three adducts are typically observed: $[M+H]^+$, $[M+C_2H_5]^+$, and $[M+C_3H_5]^+$. PCI data were imported in Compound Discoverer software and reprocessed to detect the characteristic adducts. As an example, the Compound Discoverer software results showing the PCI spectra of *p*-cymene are reported in Figure 5. The PCI workflow embedded in the software allowed the prediction of the chemical formula for the unknown compounds and assignment of the compound annotation based on multiple sources such as mzCloud™ or ChemSpider™. The presence of the methane adducts in the PCI spectrum confirmed *m/z* 134.10889 as the molecular ion for *p*-cymene (RT = 10.20 min) and supported the elemental composition of the proposed molecule.

**Table 2. Table of fold change of main volatile compounds constituents of *O. vulgare* samples with different geographical provenances.** In particular, sample A showed a significantly higher level of cymyl-type compounds such *p*-cymene (4-fold change), γ-terpinene (2-fold change), and thymol (3-fold change). Sample B had lower levels of cymyl-type compounds but was higher in acyclic compounds such as β-ocimene (4-fold change) and sesquiterpenes (such as germacrene D (2-fold change)). Sample C had significantly higher concentrations of β-ocimene and sequiterpenes (such as germacrene D).

| Name | RT [min] | Chemical Formula | Reference m/z | EI | | | PCI | | | Total Score | Log2 Fold Change | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | Measured *m/z* | Theoretical m/z | Mass error (±5 | $[M+H]^+$ | $[M+C_2H_5]^+$ | $[M+C_3H_5]^+$ | | Sample A / Sample C | Sample B / Sample C | Sample B / Sample A |
| *α*-Thujene | 8.64 | C10H16 | 91.05417 | 136.12463 | 136.12465 | -0.1 | 137.13254 | 165.16379 | 177.16380 | 93.4 | 4.0 | 3.3 | -0.7 |
| *α*-Pinene | 8.79 | C10H16 | 91.05423 | 136.12469 | 136.12465 | 0.3 | 137.13252 | 165.16377 | 177.16377 | 93.4 | 3.4 | 3.0 | -0.4 |
| *p*-Cymene | 10.21 | C10H14 | 119.0856 | 134.10892 | 134.10900 | -0.6 | 135.11688 | 163.14818 | 175.14815 | 96.2 | 3.7 | 2.8 | -0.9 |
| *γ*-Terpinene | 10.84 | C10H16 | 91.05424 | 136.12457 | 136.12465 | -0.6 | 137.13234 | 165.13659 | 177.16353 | 95.2 | 2.3 | 2.6 | 0.3 |
| β-Ocimene | 11.40 | C10H16 | 93.06971 | 136.12466 | 136.12465 | 0.1 | 137.13266 | 165.16393 | 177.16391 | 90.2 | -4.4 | -0.6 | 3.9 |
| Camphor | 12.09 | C10H16O | 95.08548 | 152.11957 | 152.11957 | 0.0 | 153.12727 | 181.15852 | 193.15848 | 96.6 | 0.6 | 1.1 | 0.5 |
| Thymoquinone | 13.54 | C10H12O2 | 149.0596 | 164.08311 | 164.08318 | -0.4 | 165.09077 | 193.12198 | 205.12195 | 94.4 | 0.1 | 0.4 | 0.3 |
| Methyl thymyl ether | 13.61 | C11H16O | 149.0962 | 164.11960 | 164.11957 | 0.2 | 165.12726 | 193.15863 | 205.15863 | 97.4 | 1.5 | 2.0 | 0.4 |
| Thymol | 14.23 | C10H14O | 135.0804 | 150.10382 | 150.10392 | -0.6 | 151.11169 | 179.14310 | 191.14310 | 96.1 | 2.8 | -0.3 | -3.1 |
| Carvacrol | 14.42 | C10H14O | 135.0805 | 150.10384 | 150.10392 | -0.5 | 151.11163 | 179.14302 | 191.14294 | 95.7 | 0.3 | 0.2 | 0.0 |
| Eugenol | 15.36 | C10H12O2 | 164.0831 | 164.08321 | 164.08318 | 0.2 | 165.09100 | 193.12228 | 205.12231 | 96.9 | -1.5 | 0.2 | 1.7 |
| Methyleugenol | 16.02 | C11H14O2 | 178.0989 | 178.09885 | 178.09883 | 0.1 | 179.10660 | 207.13788 | 219.13788 | 96.2 | -2.6 | 0.2 | 2.9 |
| *γ*-Elemene | 17.00 | C15H24 | 189.1639 | 204.18726 | 204.18725 | 0.0 | 205.19524 | 233.22658 | 245.22647 | 92.1 | 0.5 | 0.2 | -0.3 |
| *β*-Caryophyllene | 17.15 | C15H24 | 91.05417 | 204.18721 | 204.18725 | -0.2 | 205.19489 | 233.22615 | 245.22627 | 95.3 | 0.5 | -0.1 | -0.6 |
| Humulene | 17.76 | C15H24 | 93.06991 | 204.18729 | 204.18725 | 0.2 | 205.19513 | 233.22646 | 245.22649 | 94.5 | 1.8 | -0.1 | -1.9 |
| Isoledene | 18.06 | C15H24 | 105.0699 | 204.18713 | 204.18725 | -0.6 | 205.19519 | 233.22652 | 245.22665 | 96.2 | 1.2 | 0.9 | -0.3 |
| Germacrene D | 18.22 | C15H24 | 147.1167 | 204.18727 | 204.18725 | 0.1 | 205.19514 | 233.22649 | 245.22647 | 95.5 | -0.9 | 0.9 | 1.7 |
| Alloaromadendrene | 18.58 | C15H24 | 91.05424 | 204.18716 | 204.18725 | -0.4 | 205.19485 | 233.22614 | 245.22618 | 95.8 | -0.6 | 0.7 | 1.3 |
| *γ*-Muurolene | 18.78 | C15H24 | 161.1327 | 204.18719 | 204.18725 | -0.3 | 205.19499 | 233.22635 | 245.22636 | 93.6 | -0.3 | 0.2 | 0.5 |
| Isospathulenol | 19.94 | C15H24O | 91.05419 | 220.18230 | 220.18217 | 0.6 | 221.19000 | 249.22171 | 261.22125 | 94.5 | -1.3 | 0.0 | 1.3 |
| Caryophyllene oxide | 20.10 | C15H24O | 91.05419 | 220.18199 | 220.18217 | -0.8 | 221.18999 | 249.22130 | 261.22129 | 94.7 | -0.2 | -0.3 | -0.1 |

A




B

GC CI Compounds | ChemSpider Results | Mass List Search Results | Input Files | Study Information

| | Name | Formula | RT [min] | Annot. Source: Predicted Compositions (ChemSpider Search, MassList Search) | # Adducts | Annot. ΔMass [ppm] | Molecular Weight | Reference m/z |
|---|---|---|---|---|---|---|---|---|
| 83 | p-cymene | C10 H14 | 10.154 | | 5 | -0.38 | 134.10950 | 93.06992 |

**Figure 5. Compound Discoverer software results showing the PCI spectrum for *p*-cymene (RT = 10.15 min) (A) and the results table (B).** The typical adducts formed when methane gas is used are labeled in the spectrum plot in green. The annotation sources (ChemSpider and Mass List) used to propose the chemical formula for *p*-cymene, as well as the number of adducts found, the mass accuracy (in ppm), the molecular weight and the reference *m/z*, are listed in the table.

## Conclusions

The results presented in this study demonstrate that the Thermo Scientific Orbitrap Exploris GC 240 mass spectrometer in combination with SPME Arrow technology and Compound Discoverer 3.2 software represents an integrated omics approach for the characterization of the volatile fraction of food samples.

- Flavor profiling is a challenging analysis as the sample matrices encountered are chemically complex, the compounds are present over a wide dynamic range, and profiling requires sensitive and stable systems.
- Significant differences in the oregano chemotypes were detected and these can be representative of the different climate where *O. vulgare* varieties were grown with the predominance of phenolic monoterpenes in plants grown in the Mediterranean area and sesquiterpenes predominant in continental regions.
- Cymyl-type compounds (*p*-cymene, *γ*-terpinene, and thymol) were predominant in sample A, whereas other samples had high levels of acyclic compounds and sequiterpenes (such as germacrene D and β-caryophyllene).

- The high resolving power and consistent sub-1 ppm mass accuracy as well as the wide linear and dynamic range lead to fast and confident characterization of a large number of compounds regardless of their concentration or matrix complexity.
- Automated headspace sampling with the SPME Arrow eliminates the need of sample preparation and speeds up the analysis.
- The streamlined GC-EI/PCI data processing workflow integrated in Compound Discoverer 3.2 software allows for multivariate statistical analysis, extraction, deconvolution, and putative identification of the unknown compounds. The EI data obtained can be used for candidate compound identification against existing commercial libraries. Importantly, as often the chemicals detected are not included in such libraries, the consistent sub-ppm mass accuracy measurements as well as the retention index information will greatly aid in the determination of the elemental composition and subsequent structural elucidation of unknown chemicals. Moreover, softer ionization such as positive chemical ionization with methane can be used to confirm the elemental composition of the molecular ion of a chemical.

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