



All faces of the Crystal



09-243-5014EN

Application Note

Essential Oil Profiling GC-FID/MSD

Introduction

An essential oil is a concentrated hydrophobic liquid containing volatile aroma compounds from plants. Essential oils are generally extracted by distillation, often by using steam. Other processes include expression, solvent extraction, absolute oil extraction, resin tapping, and cold pressing.

Gas Chromatography with double detection system : Flame Ionizations Detector (FID) and single quadrupole mass Spectrometry detector (MSD) is powerful and accurate tool for profiling the essential oil by measuring the main components of essential oils: terpenoids, aromatic hydrocarbon (arenes), aldehydes, ...etc

Capillary Gas chromatography-Mass spectrometry (GC-MS) proves to be an efficient and precise method for qualitative, as well as quantitative estimation, for almost all combinations of components in such mixtures.

Analytical methods based on GC and GC/MS operate with 30-60 meters long capillary columns. High chromatographic efficiencies are required to achieve baseline separation and quantitative determination of the important groups of components. Such methods generally require 30-60 minutes to perform an overall analytical cycle.



GC-FID can be a good starting point in this typical application field, however, sometimes unambiguous qualitative identification of some key components becomes extremely important. GC-MS with electron impact ionization (EI) offers a powerful tool for separation and identification with EI -MS library facility, which is a much more efficient technique than GC-FID for such critical requirements. Analytical challenge is high in the case of essential oils, particularly for the identification of various isomers, hence EI-MS library searches need to be complemented by retention time information in TIC chromatograms.

Experiment

Sample

The sample is essential rosemary oil prepared with steam extraction. Rosemary oil has specific composition ratio of the main components: monoterpene hydrocarbons, oxygenated monoterpenes and sesquiterpene hydrocarbons.

Instrument configuration

- Gas chromatograph Chromatec-Crystal 9000
- Split splitless inlet (SSI)
- Column 30 m × 0.25 mm
0.25 µm film
- FID detector
- MSD (EI)
- Carrier-gas – helium

Operating mode

Chromatograph

Analysis time 30 min

Column

Carrier-gas flow 1.6 ml/min

Flow split 1:150

Column temperature 40 °C for 0.5 min
40 - 150 °C at 4°C/min
150 – 270 °C at 8°C/min

Inlet

Inlet temperature 275 °C

FID detector

Hydrogen flow rate 25 ml/min

Air flow rate 250 ml/min

Make up gas flow 20 ml/min

Detector temperature 300 °C

Sample volume 0.5 µL

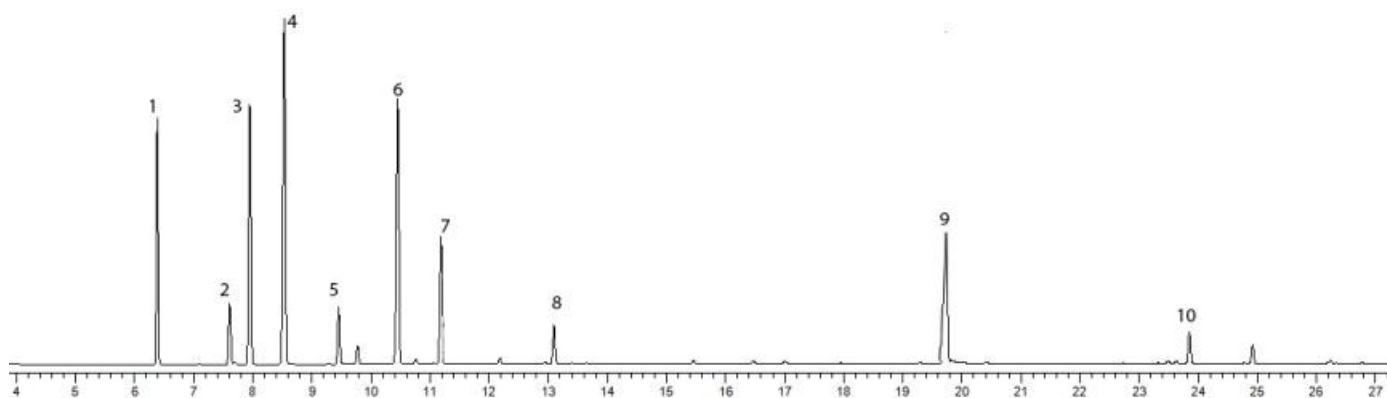
MSD

Scan Range 40 – 450

Ion Source 230 °C

Chromatograms

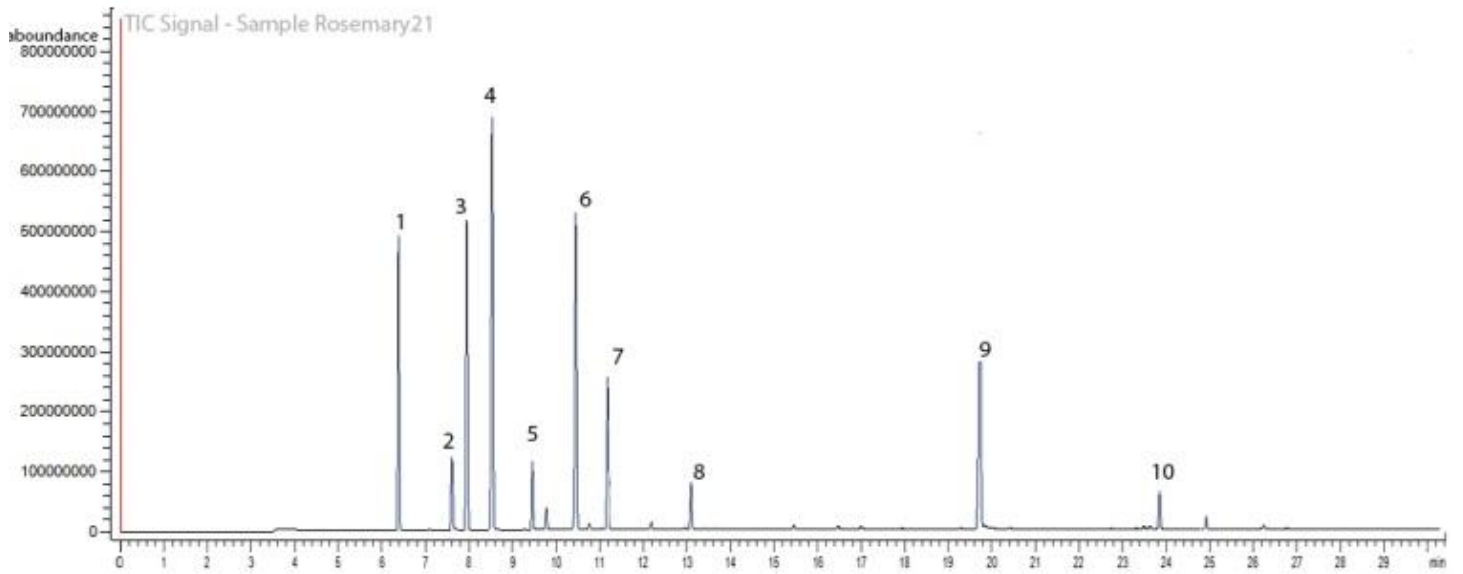
Rosemary Oil FID Chromatogram:



1. α-Pinene
2. Camphene
3. β-Pinene
4. Limonene
5. Linalool

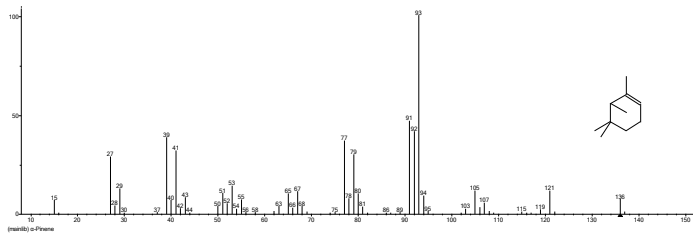
6. Camphor
7. Terpinene-4-ol
8. Isoborneol
9. Borneol
10. α-Terpineol

Rosemary Oil TIC:

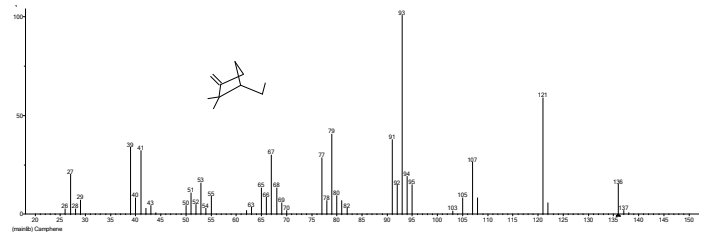


NIST2011 Library Search Results:

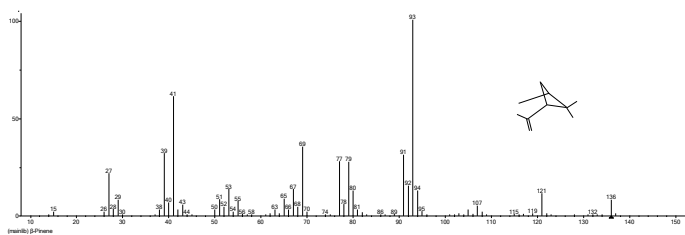
1. α -Pinene Spectra:



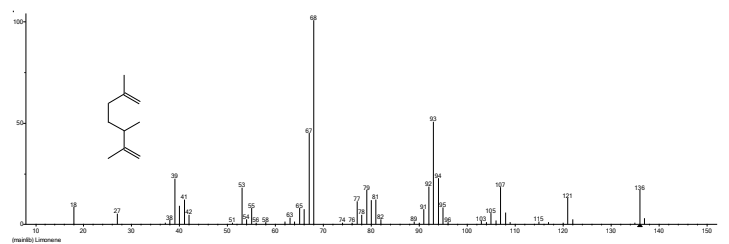
2. Camphene



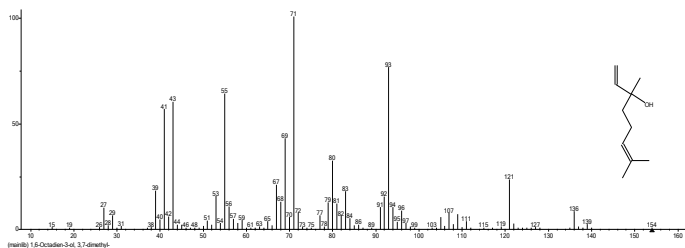
3. β -Pinene



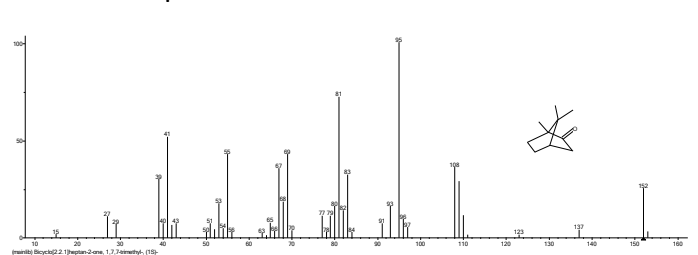
4. Limonene



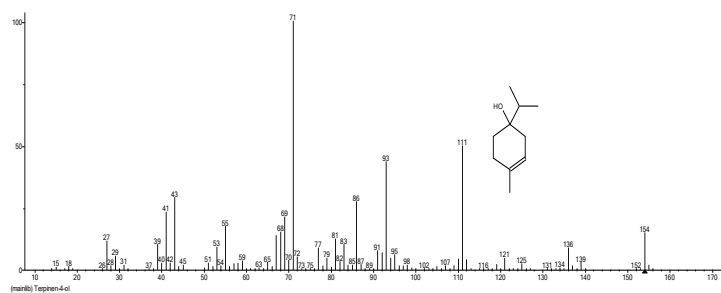
5. Linalool



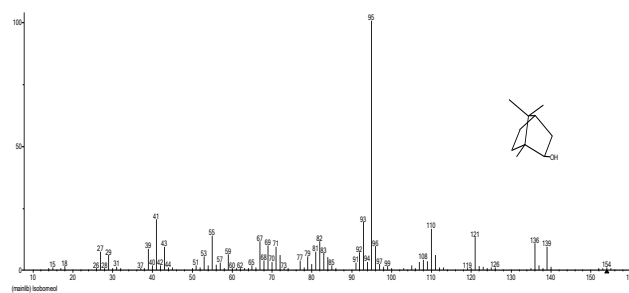
6. Camphor



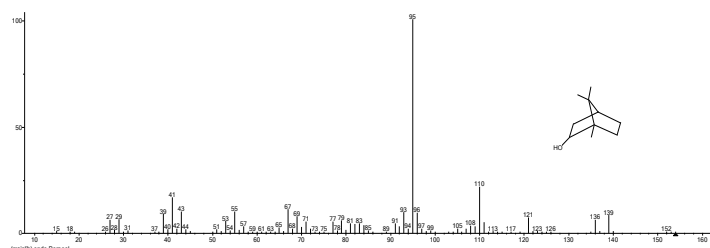
7. Terpinene-4-ol



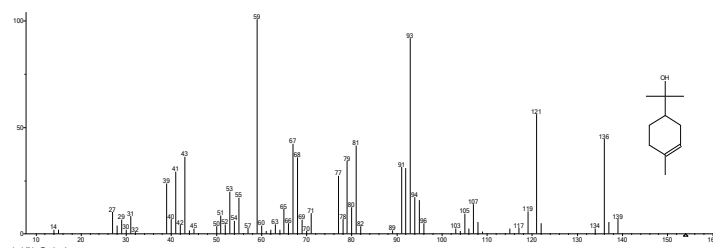
8. Isoborneol



9. Borneol



10. α -Terpineol



Conclusion:

This application successfully demonstrated reliable analysis and fingerprinting of rosemary oil using Chromatec GC with both FID and GC/MSD detection. Peaks of interest at or above the 0.25% by area level were identified by GC/MS and labeled in a corresponding GC-FID chromatogram with the same separation. Once the fingerprinting and identification of the peaks of interest are established, characterization of subsequent samples by GC-FID is straightforward. This two-step approach helps to characterize these complex samples quickly and cost-effectively.

The data provided herein can be changed without prior notice.
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