

Instrument: Pegasus[®] BTX

Characterization and Comparison of Lavandin Essential Oil Aroma Profiles by Using Fast GC-TOFMS and ChromaTOF[®] Sync

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Introduction

The qualitative characterization of essential oil volatiles is commonly performed using GC-MS; however, conventional methods often rely on long capillary columns, slow oven temperature ramps, and helium as the carrier gas. These factors typically result in analysis times exceeding one hour, higher operational costs, and limited sample throughput. Detailed aroma profiling, such as for lavandin essential oil, is nonetheless critical for understanding complex chemical composition, identifying key aroma-active compounds, and assessing compositional variability between samples.

Fast GC-TOFMS, using hydrogen (H_2) as the carrier gas, offers an effective solution for the rapid analysis of complex essential oil matrices. Optimized temperature programming and high oven heating rates significantly reduces analysis time while maintaining chromatographic resolution. The Pegasus BTX GC-TOFMS system generates highly detailed datasets, which are efficiently processed using ChromaTOF Sync software for automated peak detection, chromatographic alignment, and non-targeted comparison across multiple samples. Here three lavandin oil varieties (Lavandin Oil Abrialis, Grosso, and Super) were analyzed and compared using this workflow to investigate compositional differences and identify discriminant compounds, with selected results highlighting some relevant findings.



Experimental

Three varieties of lavandin essential oil samples, namely Abrialis, Grosso, and Super, were analyzed using fast GC-TOFMS after appropriate dilution in n-hexane. The instrumental conditions are reported in Table 1.

Table 1. Experimental Conditions

Autosampler	LECO L-PAL 3 Autosampler
Injection	0.2 μ L, Split 200:1
Gas Chromatograph	Agilent 8890 Gas Chromatograph
Inlet	250 °C
Column	Rxi-5 Sil MS 20 m x 0.18 mm x 0.18 μ m (Restek)
Carrier Gas	Hydrogen, 1.26 mL/min, constant flow
Oven Program	50 °C (0.1 min), 20 °C/min to 325 °C
Transfer Line	300 °C
Mass Spectrometer	LECO Pegasus BTX
Ion Source	250 °C
Mass Range	40–450 m/z
Acquisition Rate	20 spectra/s

Results and Discussion

Figure 1 shows the overlaid chromatograms of the lavandin essential oil samples.

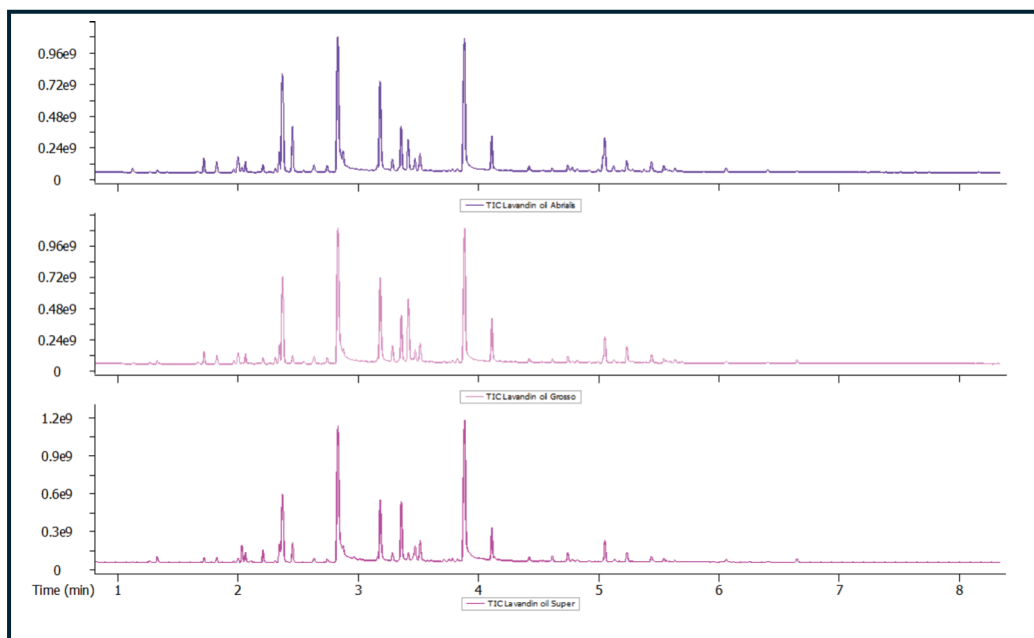


Figure 1. Overlaid total ion chromatograms from three different lavandin essential oils.

The use of H₂ carrier gas and fast oven temperature programming enabled a rapid GC-TOFMS method with total analysis times of less than ten minutes while maintaining adequate chromatographic separation. Lavandin essential oil was found to be dominated by oxygenated monoterpenes and their esters, with linalool and linalyl acetate as the most abundant constituents contributing to its characteristic floral and herbaceous aroma. Additional compounds of interest, typically used for authenticity verification or quality control were also detected, including lavandulol, lavandulyl acetate, and geranyl acetate.

Fast GC-TOFMS generated detailed chemical profiles that were efficiently processed using *ChromaTOF Sync* software, allowing automated peak deconvolution, alignment, and comparison across samples. This approach enabled rapid identification of compositional similarities and differences, including a major compound identified with high confidence.

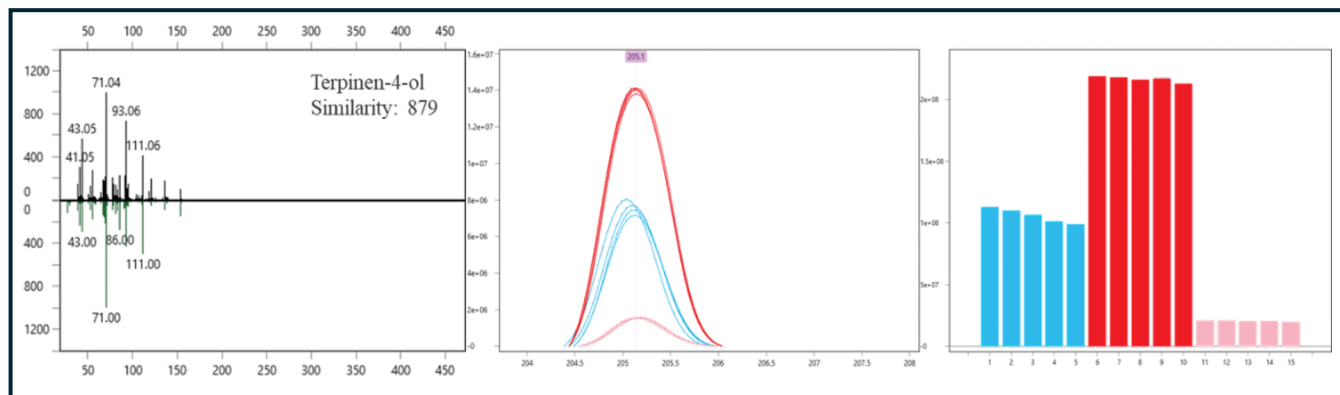


Figure 2. Spectral information, overlaid chromatographic profiles, and relative trends (bar graph) of terpinen-4-ol.

Terpinen-4-ol exhibited a highly significant difference among the sample groups ($p < 0.001$), underscoring its potential role in discriminating lavandin essential oil samples. The compound was identified with a mass spectral similarity score of 879 matched against the FFNSC 4 library database, and its distribution across the samples is illustrated through overlaid chromatograms and bar graphs of relative peak areas (Figure 2). Specifically, lavandin Grosso (red) exhibits the highest abundance, followed by lavandin Abrialis (light blue), while lavandin Super (pink) shows the lowest levels.

Conclusions

This application note demonstrates that fast GC-TOFMS using the Pegasus BTX system is a powerful and reliable solution for the rapid characterization of lavandin essential oils. The use of H_2 and fast temperature programming dramatically reduces run time while maintaining analytical performance.

The integration of ChromaTOF Sync is critical for handling complex datasets, enabling efficient peak alignment, non-targeted profiling, and robust comparison of multiple samples. Together, this workflow supports rapid aroma profiling, identification of key discriminant compounds, and confident differentiation of lavandin essential oil varieties.