Automated Chromatographic Comparison of Citronella Ceylon Oils Using GC-TOFMS

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Key Words: GC-TOFMS

1. Introduction

Citronella ceylon oil is a complex mixture of volatile and semi-volatile organic components. The oil is used in a variety of household products from soaps to aerosols. Minor differences in the composition of ceylon oils from different regions can greatly affect their scent and it is important to detect variations in the oils in order to ensure that the commercial product is manufactured consistently over time.

The LECO Pegasus® II GC-TOFMS offers a unique comparison algorithm, which automatically locates and identifies minor differences between two samples or between an unknown sample and a reference standard. The peak find algorithm effectively locates the position of all peaks in each of the samples including multiple components in complex coelutions. The deconvolution algorithm resolves the mixed mass spectra of the coelution into accurate individual mass spectra for each analyte, including the accurate distribution of signal from masses shared by several components in the coelution. Once the peaks are located and the spectra determined for each sample, the comparison is performed based upon peak positions and spectral similarities. Components present in one sample and not in another are identified as well as components present in both samples, but at widely varying concentrations (based upon a user-defined threshold).

2. Experimental Conditions

Two samples of ceylon oil were analyzed. Automated data processing was performed with peak finding and spectral deconvolution. The resulting mass spectra were searched against both the National Institute of Standards and Technology (NIST) 1998 Mass Spectral Database and the Terpene Essential Oil Library.[1]

Detector:
LECO Corporation Pegasus II Time-of-Flight Mass Spectrometer

Transfer Line:	300°C
Source:	200°C
Acquisition Rate:	30 spectra/second
Stored Mass Range:	35 to 400 u
GC:	Hewlett Packard® 6890*

Column:
DB-5 4 m x 0.1 mm ID, 0.1 µm phase film

Oven:
40°C for 0.5 minute, then to 280°C at 75°C/minute, hold for 1 minute

Injector:	Split/Splitless at 290°C
Carrier Gas:	Helium, 2.0 ml/minute constant flow
Sample:	No preparation required; 0.1 µL split (150:1) injection.

**HP6890 GC is equipped with fast oven temperature ramp capabilities and a high pressure EPC module.*

3. Results

Based upon the Total Ion Chromatogram overlay (Figure 1), the samples appear very similar. However, the comparison algorithm was able to detect a peak present in ceylon 1 that is not in ceylon 2 and is essentially below the baseline of the TIC. Table 1 lists the difference found between the samples and Figure 2 highlights the TIC in the expanded region of the difference. Even in the expanded view it is difficult to visually detect the difference. However, the comparison algorithm has detected a difference in this region. By plotting the unique mass, m/z 58, determined by the algorithm (Figure 3), the component that differs in the two samples is readily apparent. The acquired mass spectrum for the additional component in ceylon 1 is shown in Figure 4 in addition to the library spectrum for the analyte.

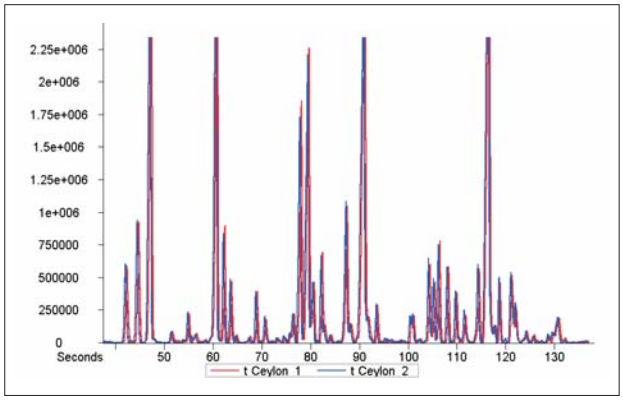

Figure 1. Total Ion Chromatogram Overlay (TIC) of Ceylon 1 and Ceylon 2.

Table 2. Ceylon Comparison Peak Table.

Peak	*Name*	*R.T. (sec.)*
47	2-Undecanone	94.690

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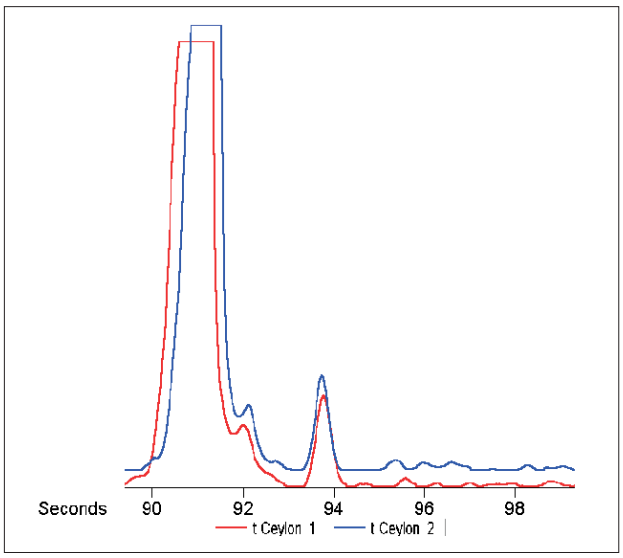

Figure 2. Expanded Total Ion Chromatogram (TIC) Overlay of Ceylon 1 and Ceylon 2.

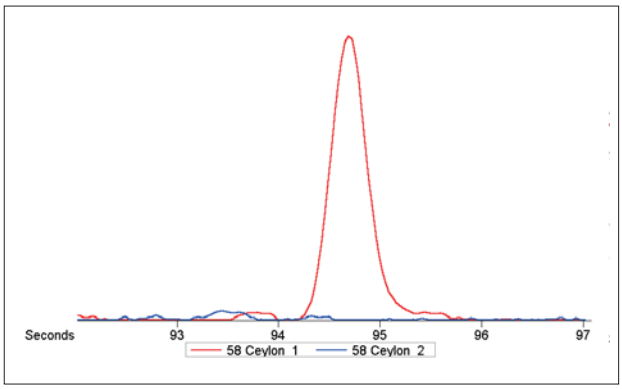

Figure 3. Extracted Ion Profile Chromatogram Overlay of m/z 58 in Ceylon 1 and Ceylon 2.

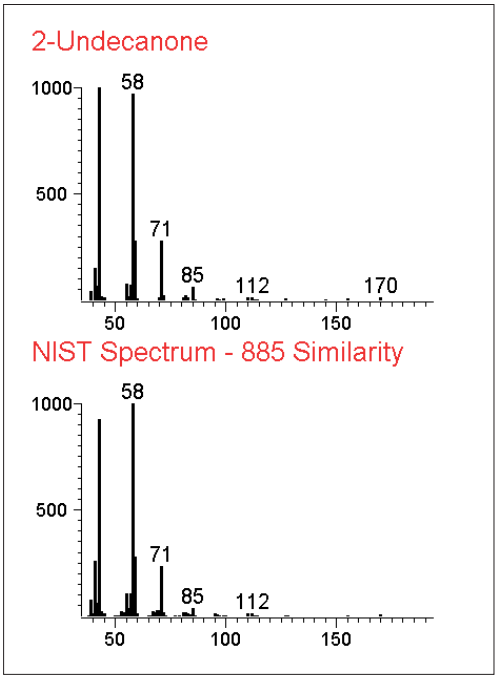

Figure 4. Mass Spectrum for component present in Ceylon 1 and not in Ceylon 2.

4. Conclusions

The combination of unique peak find and spectral deconvolution algorithms along with an automated sample comparison routine allow for the rapid identification of even minor differences between samples of similar composition with the Pegasus II GC-TOFMS.

5. References

[1]The Terpene Library contains mass spectra of essential oil components and DB-5 retention indices compiled by Robert P. Adams, Baylor University Plant Biotechnology Center.

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