Profiling of Essential Oil VOCs and SVOCs by GC-TMS

Spice and fragrance essential oil raw materials frankin-cense (Boswellia carterii) from India and Somalia, sandalwood (Santalum album) from India and Indonesia, and corn mint (Mentha haplocalyx) from the United States were analyzed for on-site analytical profiling and confirmation of quality and purity of therapeutic grade essential oils from raw materials. A novel coiled wire fil-ament (CWF) was used to inject ~1 ≒L of sample extract into a portable gas chromatograph-toroidal ion trap mass spectrometer (GC-TMS).

Introduction

Acceptance of raw materials in food and fragrance indus-tries historically is performed by sensory evaluation (taste, smell, appearance) without definitive analytical data to support quality control. Portable analytical instruments for on-site characterization by chromatography/mass spec-trometry have only recently become available. Product-specific volatile and semivolatile organic compounds (VOCs, SVOCs) can be used to verify the identification, source, or quality of a commodity. For rapid screening, a product profile containing marker compounds can be created to match against a new lot of material prior to acceptance. This pre-acceptance approval process has numerous benefits including decreased rejection rates due to counterfeit/bait-and-switch products. Coiled wire fila-ment (CWF) sampling combined with portable gas chroma-tography-toroidal ion trap mass spectrometry (GC-TMS) is an effective tool for on-site analysis of VOCs and SVOCs at the point of origin or upon receipt of a commodity.

Experimental Conditions

Frankincense, sandalwood and corn mint were provided by Rocky Mountain Oils (Springville, Utah). Essential oil extracts were prepared by dissolution in dichloromethane (~1% v/v). Sampling was performed by placing the CWF into the sample solution, with ~1 ≒L uptake by capillary action. The solvent was evaporated in air for 5 s, and the CWF syringe was inserted into the TRIDION™-9 GC-TMS injection port, desorbing the target analytes into a low thermal mass injec-tor (270°C) coupled with a capillary GC column (MXT-5, 5 m x 0.1 mm, 0.4 µm d_f [Restek, Bellefonte, PA]). After an initial 30 s hold at 40ºC, the GC temperature was increased at 0.3°C/s to 250ºC, with a final hold for 100 s. The capillary GC is coupled to a TMS detector with a mass range of 45-500 *m/z*.

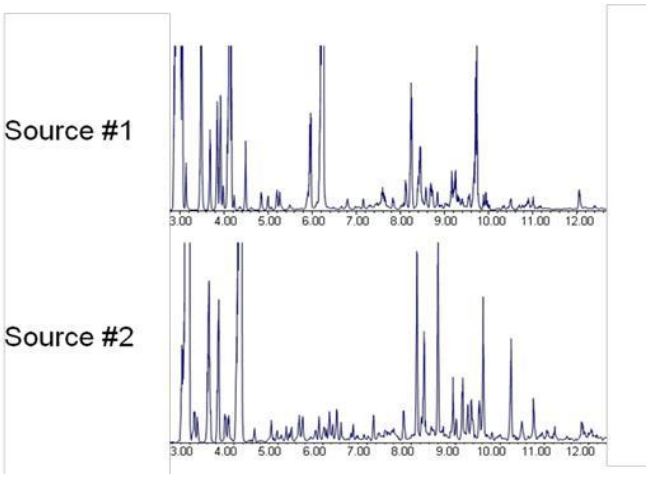

Figure 1: *Comparison chromatograms of two sources of frankincense from India and Somalia. Compound profiling readily distinguished between the sources of the essential oil raw materials.*

Results

Figure 1 shows the GC-TMS chromatograms for two differ-ent sources of frankincense. Each sample is discernibly dif-ferent based on the presence/absence of chemical com-pounds at specific retention times. Source #2 does not con-tain major compounds found at 6 min (p-allyl Anisole) and 10.2 min (caryophyllene oxide). Likewise, caryophellene (8.6 min) in source #2 is not found in as appreciable an amount in source #1. This likely indicates that the samples are either from different sources, or that the original lot has undergone atypical aging or improper storage.

Conclusions

VOCs and SVOCs from essential oils can be quickly analyzed on-site using GC-TMS. Profiling of these compounds using the TRIDION-9 GC-TMS can support acceptance decisions of commodities at the source. The short GC-TMS analysis time allows the user to quickly analyze and evaluate multiple samples. VOC and SVOC marker screening can be used to verify raw material quality and/or identification.

References

1. EPA SW-846 Method 3815 *Screening Solid Samples for Volatile Organics*, Revision 0, February 2007, http://www.epa.gov/ epawaste/ hazard/test methods/sw846/pdfs/3815.pdf
2. Zhang, Zhouyao; Pawliszyn, Janusz. *Analysis for organic compounds in environmental samples by headspace solid phase microextraction*. Journal of High Resolution Chromatography (1993), 16(12), 689-92.

Acknowledgements

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