



Profiling of Essential Oil VOCs and SVOCs by GC-TMS

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*Spice and fragrance essential oil raw materials frankincense (*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 filament (CWF) was used to inject ~1 μ L of sample extract into a portable gas chromatograph-toroidal ion trap mass spectrometer (GC-TMS).*

Acceptance of raw materials in food and fragrance industries 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 spectrometry 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 filament (CWF) sampling combined with portable gas chromatography-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, UT). 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 μ L uptake by capillary action. The solvent was evaporated in air for 5 s, and the CWF syringe was inserted into the GUARDION®-7 GC-TMS injection port, desorbing the target analytes into a low thermal mass injector (270 °C) coupled with a capillary GC column (MXT-5, 5 m \times 0.1 mm, 0.4 μ m d_f [Restek, Bellefonte, PA]). After an initial 30 s hold at 40 °C, the GC temperature was increased at 0.3 °C/s to 250 °C, 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.

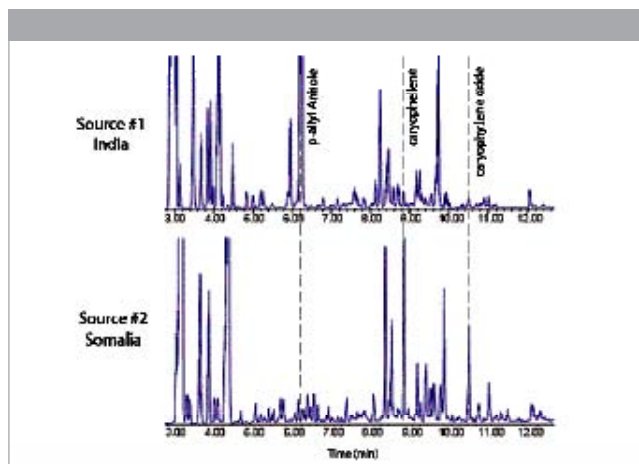


Figure 1: Comparison chromatograms of two sources of frankincense from India and Somalia. Compound profiling readily distinguished between the sources of the essential oil raw materials.

Results

Figure 1 shows the GC-TMS chromatograms for two different sources of frankincense. Evident from the chemical profiles, each sample is discernibly different based on the presence/absence of chemical compounds at specific retention times. For example, source #2 does not contain major compounds found at 6 min (p-allyl Anisole) and 10.2 min (caryophyllene oxide) found in source #1. Likewise, the compound at 8.6 min (caryophellene) in source #2 is not found in as appreciable an amount as source #1. Under quality control, 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 rapid GC-TMS. Using the GUARDION-7 GC-TMS, profiling of volatile and semi-volatile compounds 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 on-site. VOC and SVOC marker screening can be used to quickly verify raw material quality and/or identification.

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