Essential Oils Analyzed by GC-IR

Essential oils of plants from every corner the world are the foundation for many fragrance, flavoring and "nutriceutical" products found in the marketplace. Often the chemicals which give an oil its distinctive qualities are low in abundance compared to the most prevalent species, and can be very similar in structure to components known from related oils previously analyzed. Analysis of these natural products can challenge the state of the art in the analytical lab. **Infrared spectral analysis** can provide a complementary, "orthogonal" detection method that can lend greater confidence to the identification process. This brief note demonstrates the ability to discriminate among structural isomers by IR spectra alone.

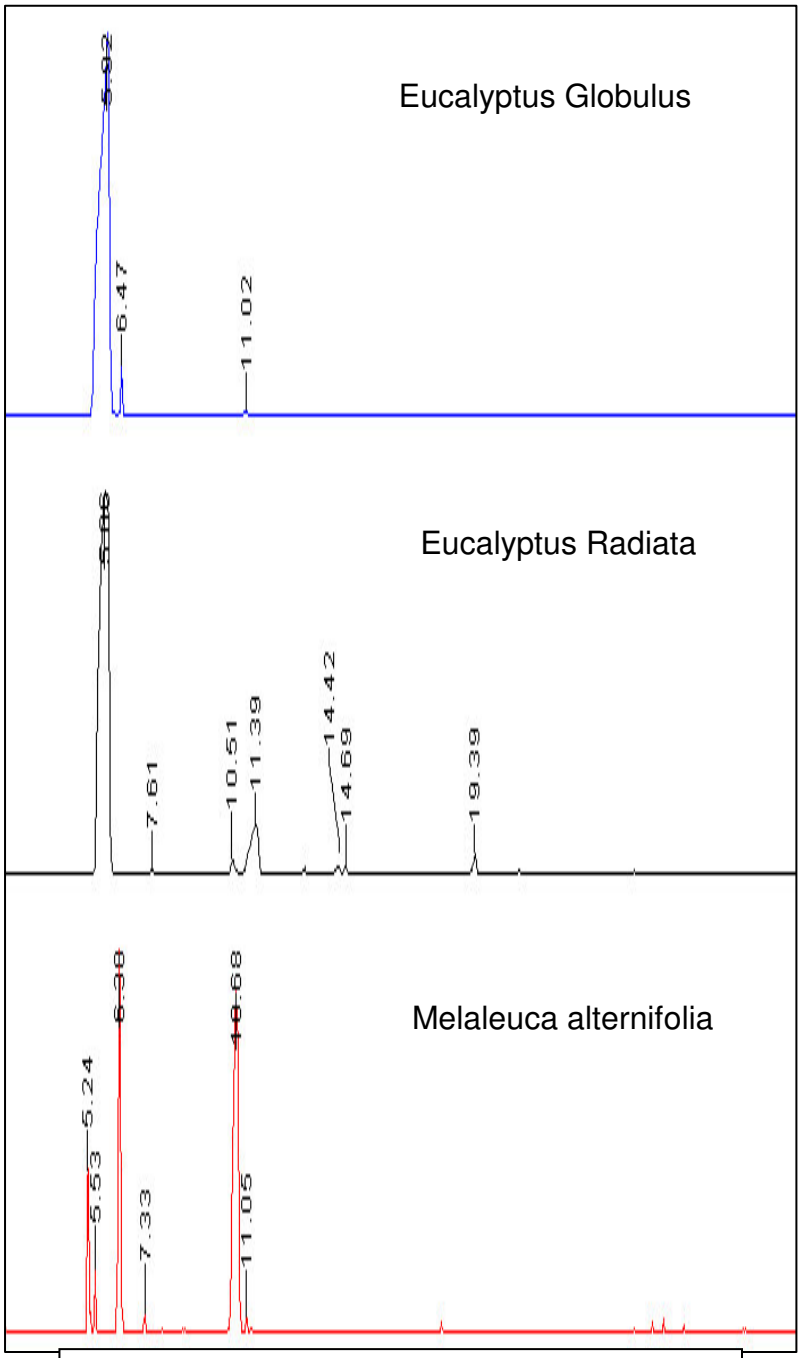
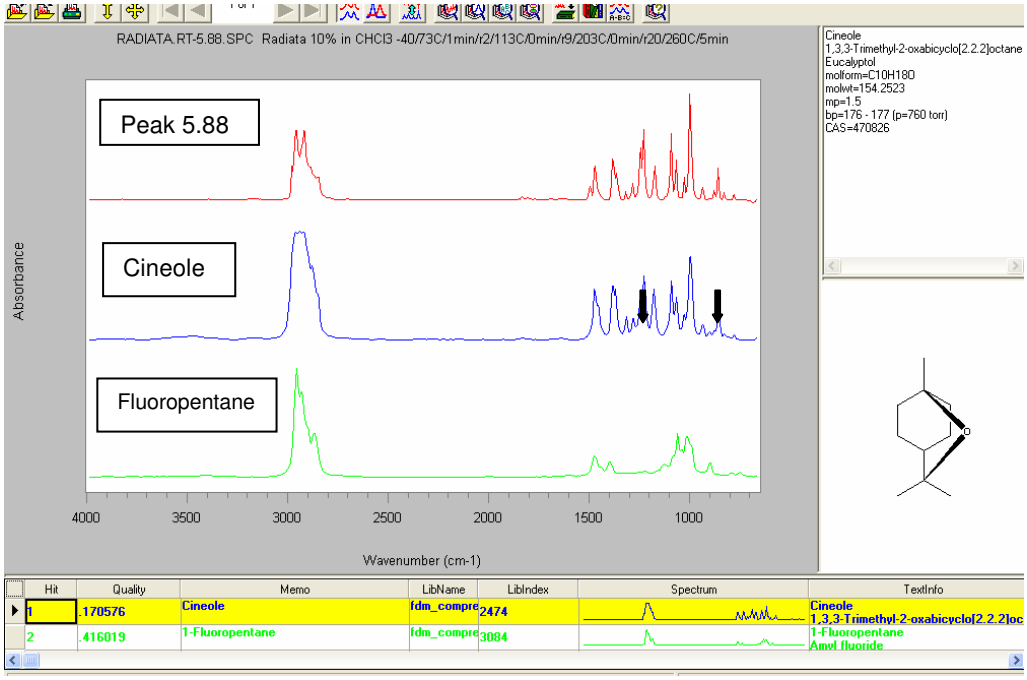


Fig. 1: Spectral Maximum Chromatograms of Essential oils

For this series of analyses, three Essential Oils [Eucalyptus globulus, Eucalyptus radiata, & Melaleuca alternifolia (tea tree oil)] were analyzed by deposition and IR detection after separation GC on a standard DB-5 column. Each exhibits a distinctive pattern as a Spectral Maximum Chromatogram (**SMC**) that plots peaks of highest IR absorbance across all wavelengths. The DiscovIR–GC™ system automatically generates full IR spectra for each peak. Comparison of the spectra to the solid-phase IR libraries by the DiscovIR™ software yields proposed chemical ID's that correspond to the data from GC-MS analysis

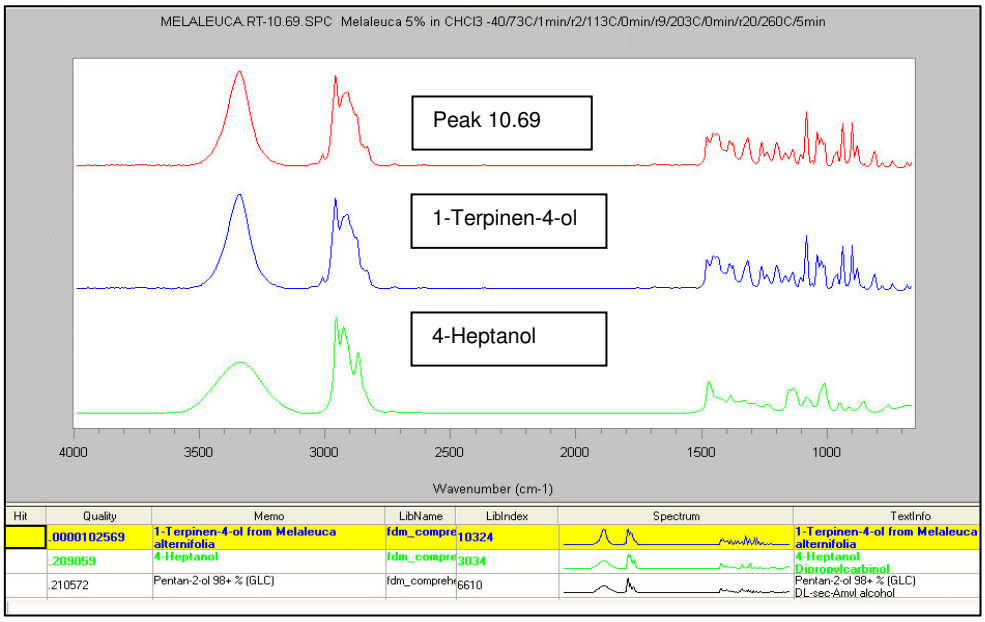
Compound Search using DiscovIR's Infrared library

Cineole



Using the peak from E. radiata which elutes a 5.88 minutes (and corresponds to peaks in E. globulus & M. alternifolia), the library shows an overall good pattern match with Cineole.

The 10.69 peak from M. Alternifolia was not found in the standard library that comes with the DiscovIR™ system. Research into additional IR libararies along with MS data gave a strong ID of 1-Terpinen-4-ol. The spectrum was easily added to the DiscovIR™ library so future analyses would display this result.



1-Terpinen-4-ol

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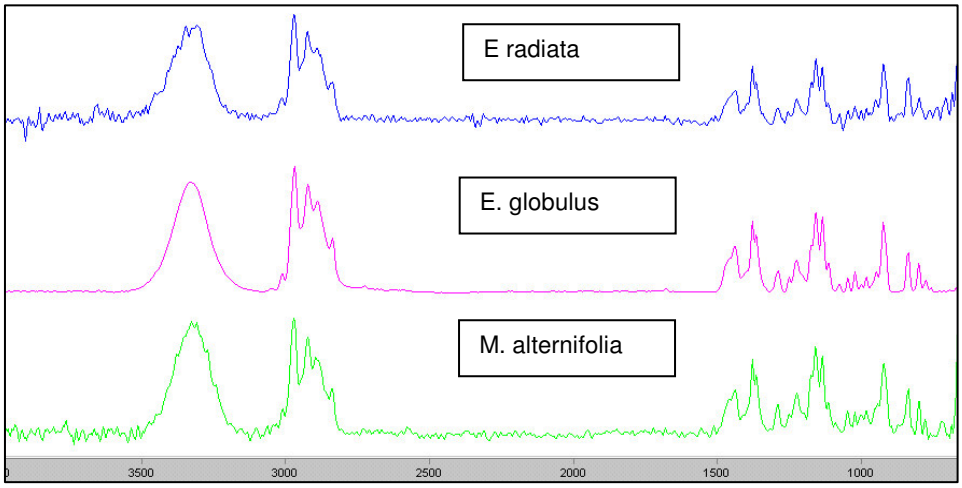
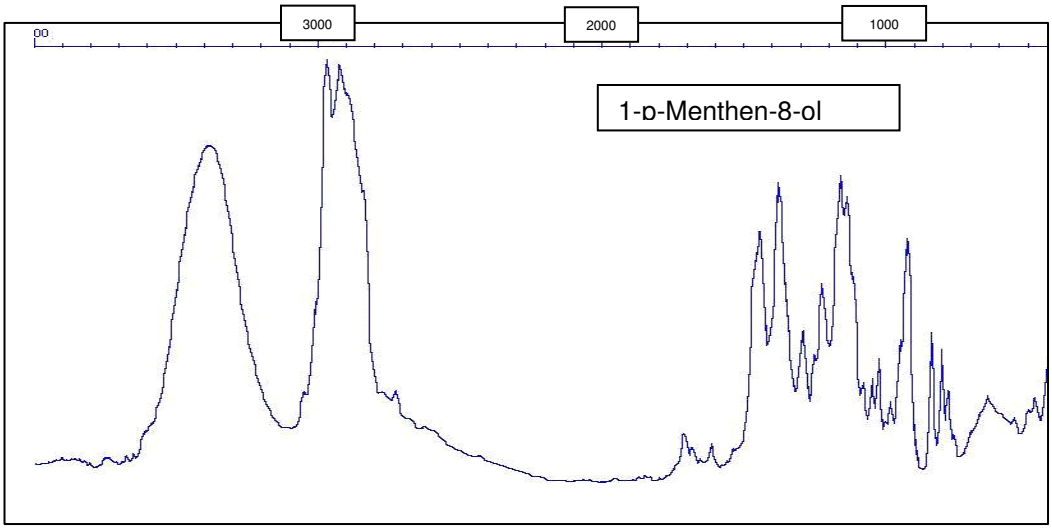


The three spectra here come from corresponding peaks from the three oils. E. radiata 11.39

The peaks from E. globulus at 11.02 min & M. alternifolia 11.05 are relatively small peaks (see figure 1), but the spectra here are of equal quality to the more substantial peak of E. radiata.



This spectrum of 1-p-menthen-8-ol from the literature corresponds closely to those above. Mass data from GC-MS confirms the assignment.

The data above are from the real-time deposition and detection procedure, even though the peaks are minor species, demonstrating the sensitivity of the system. An added feature of The DiscovIR™ System is the capability to re-scan the deposited track as many times as necessary to reinforce the signal and build a useful spectrum from out of the random noise, providing even better sensitivity when needed.

Sample Conditions:

Sample:	Commercially available essential oils
Concentration	10% in $CHCl_3$
Injection:	1 µL using split/splitless injector, split 50:1
Column:	DB5, 20-meter x 0.32-mm ID, 0.25-µm film
Conditions:	Helium carrier, 1 mL/min
Temp program:	70^0C for 1 min, 2^0/min up to 113^0 , 9^0/min up to 203^0, 20^0/min to 260^0
Sample disc:	-40^0C

Injector, transfer line, restrictor tip all at 250^0 C

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