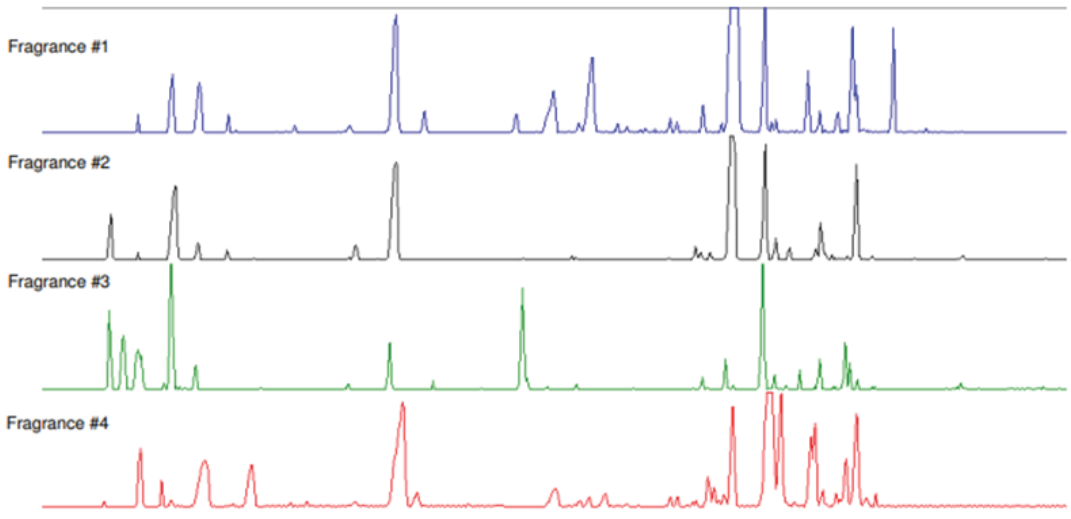
SPECTRA ANALYSIS

APPLICATION NOTE 002

Analysis of Commercial Fragrances by GC-IR

Commercial fragrances are complex mixtures of aroma compounds, solvents and fixatives. Many of these ingredients have been well-characterized through separation methods coupled to various detection modes, but this complexity can be a challenge when exhaustive analysis is required. Occasionally compounds are encountered which cannot be distinguished on the basis of just a single characteristic such as mass. In these cases, access to another detection method which provides complementary, "orthogonal" information can be extremely useful and simplify the identification process. This study demonstrates the utility of Infrared spectral analysis to discriminate among structural isomers and classify unknowns.



Four commercially available retail fragrances were analyzed by deposition and IR detection after separation GC on a standard DB-5 column. Each exhibits a distinctive pattern as a Spectral Peak Chromatogram (SpC) that plots peaks of highest IR absorbance across all wavelengths. The DiscovIR–GCTM system automatically generates full IR spectra for each peak.

Comparison of the spectra to the solid-phase IR libraries by the DiscovIRTM software can uniquely identify the unknowns. When the potent combination of Mass and IR library matching is used, structure assignments can be made with higher confidence. A key feature of Infrared analysis is that absorption at a certain wavelength is in direct proportion to the amount at hand. Therefore, relative quantities can be determined with confidence, avoiding errors due to disparity in ionization or presence of chromophores.

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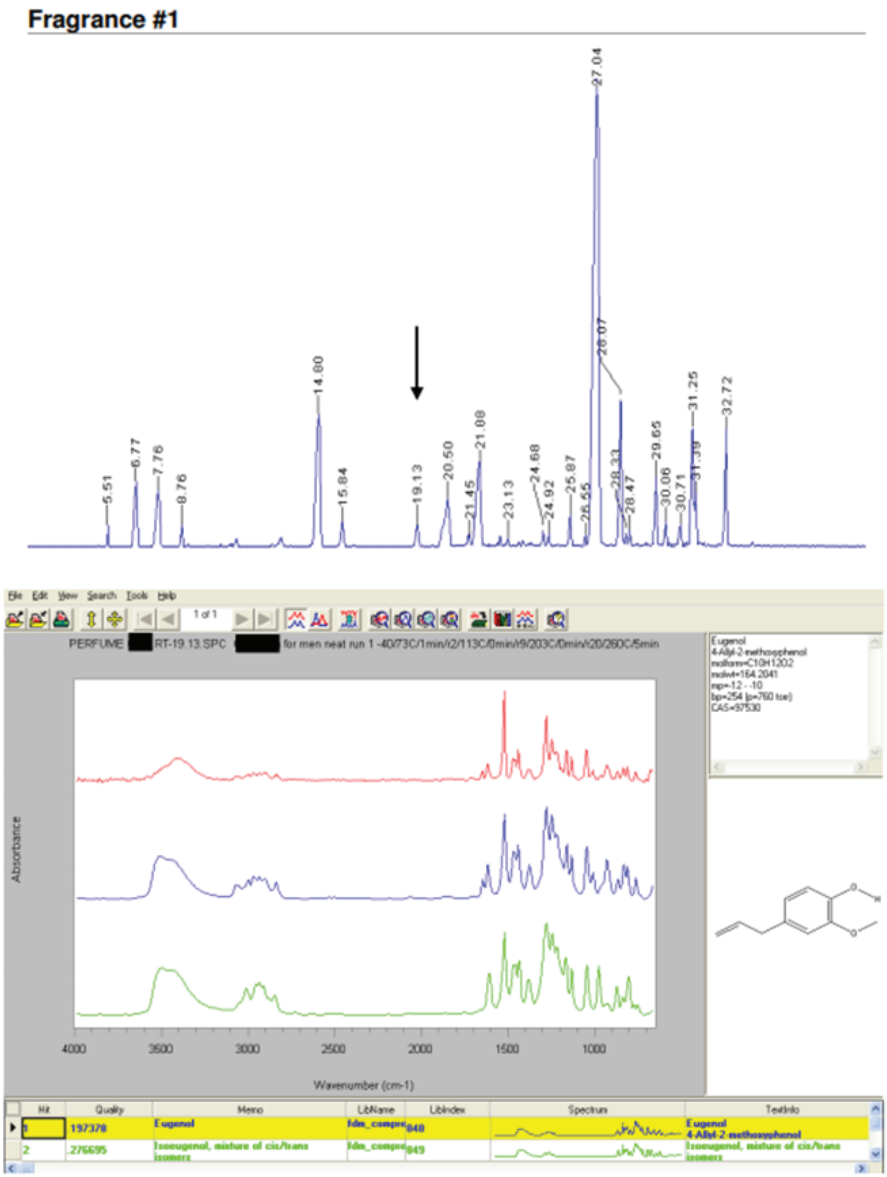
Compound Identification using Infrared library searching

Analysis of Fragrance #1 provides an example of a minor peak eluting at 19.13 minutes. Comparison of the full IR spectrum of that peak shows a close agreement to that of Eugenol as compared to Isoeugenol, leading to a good assignment.



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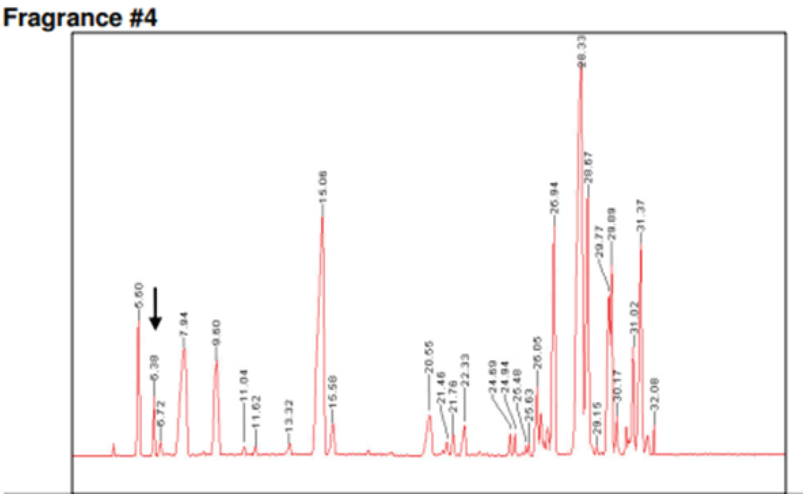
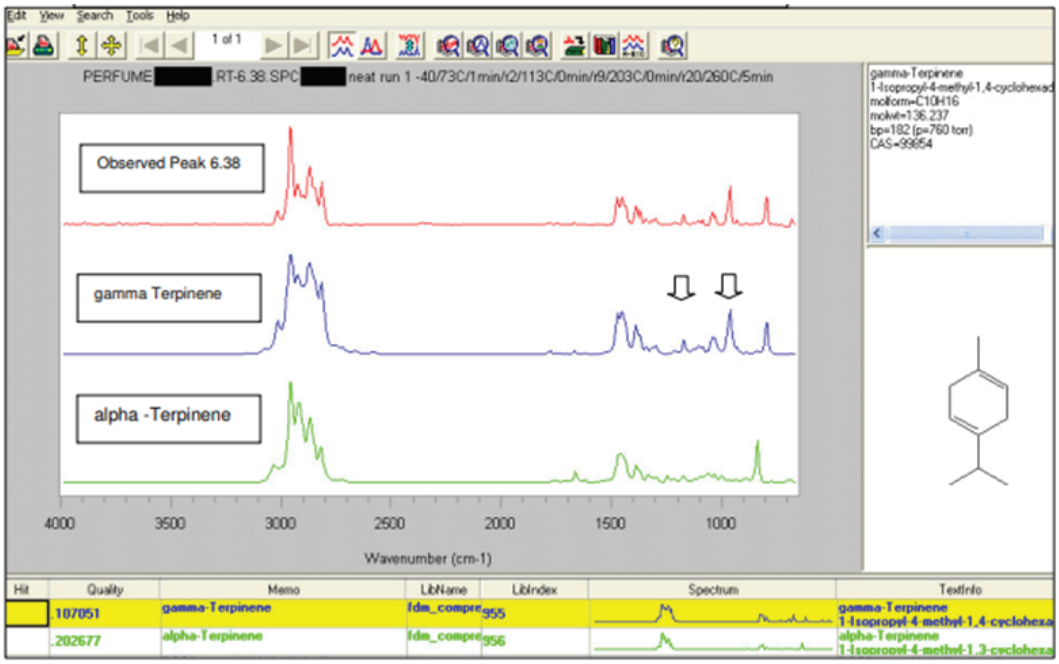
Discriminating between Structural Isomers

The peak eluting at 6.38 minutes from Fragrance #4 is an example of a compound where the orthogonal information from an IR spectra discriminates between structural isomers having the same molecular weight. The features in the 1000-1300 range identify this peak as γ-terpinene.





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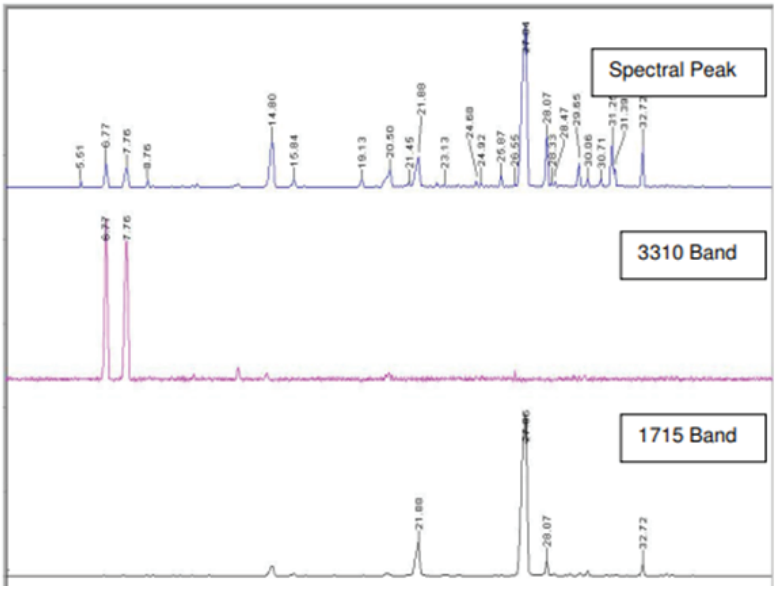
Functional Group Classification Using Band Chromatograms

Often, classification by functional groups is the analytical goal, for example when screening for a family of compounds. For this purpose, the DiscovIRTM's Band Chromatogram display is a very useful tool. A distinctive pattern of bands can be defined for a particular molecule and its related species to help recognize which peaks in a complex chromatogram are those of interest.

Fragrance #1



In the figure above, the top chromatogram displays the Spectral Peak Chromatogram, with each peak representing the maximum absorbance at any wavelength at that retention time. The middle trace shows that the peaks at 6.77 and 7.76 minutes have strong absorbance at 3310 wavenumbers, indicating that they are likely to have an alcohol functionality. The lower trace shows that the peaks at 21.88, 27.06, 28.07 and 32.72 absorb at 1715, indicating a carbonyl group, likely aldehydes or conjugated esters.

Sample Conditions:

Sample:	Four commercially available retail fragrances.
Concentration	Neat as obtained
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° for 3 min, 2°/min up to 113° C, 9°/min up to 203°, 20°/min to 260°
Sample disc:	- 40° C

Injector, transfer line, restrictor tip all at 250° C

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