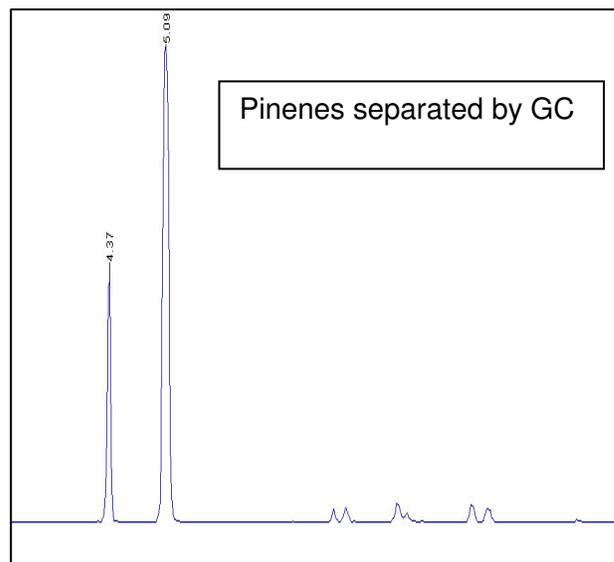


## Distinguishing Structural Isomers Using Chromatography and on-line IR Detection

Although retention time in a particular separation scheme is recognized as a reliable method for determining known analytes, an extra dimension of confidence is added when the detection method provides some corroborating structural information about the molecule. Mass spectrometry is established as the method of choice for many labs, given its resolution, sensitivity and general availability.

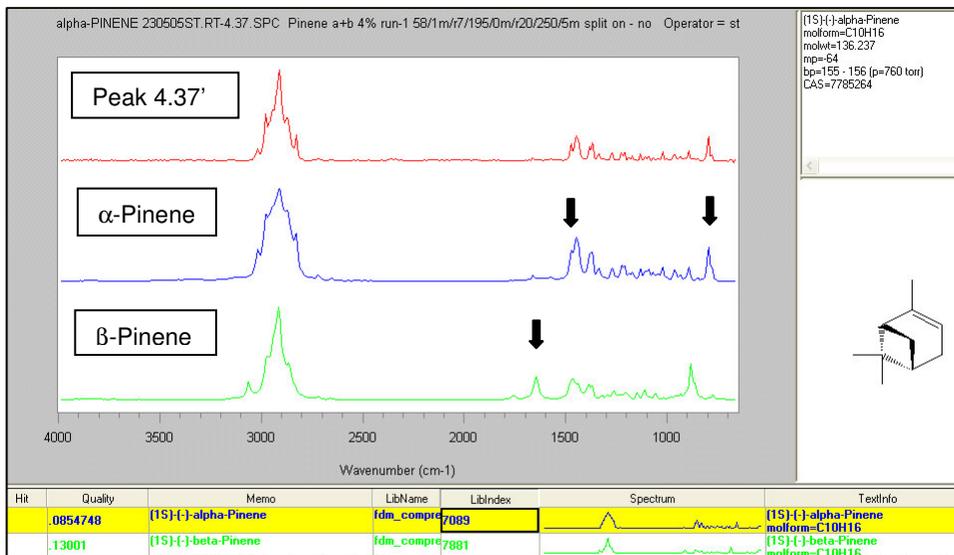
However, for structural isomers, i.e. compounds which have the same molecular weight, Mass Spec provides information that is consistent with but not diagnostic for identification, leaving retention time as the key differentiating factor. In these cases, access to another detection method which provides complementary, “orthogonal” information can be extremely practical and fortify confidence in the structural assignment. Infrared spectral analysis using the **DiscovIR™ Deposition and Detection System** makes it quick and convenient to discriminate among structural isomers. The system is designed to run independently or in parallel with a Chromatograph/Mass Spectrometer combination



The **DiscovIR-GC™ system** automatically generates full IR spectra for each peak which can be compared to the solid-phase IR libraries. The included Library of 10,000 + compounds can be expanded through access to private or commercially available libraries, and compounds can be added by the user as they are encountered. Of course, when the combination of Mass and IR Spectral Library matching is used in parallel, structure assignments can be made with very high confidence.

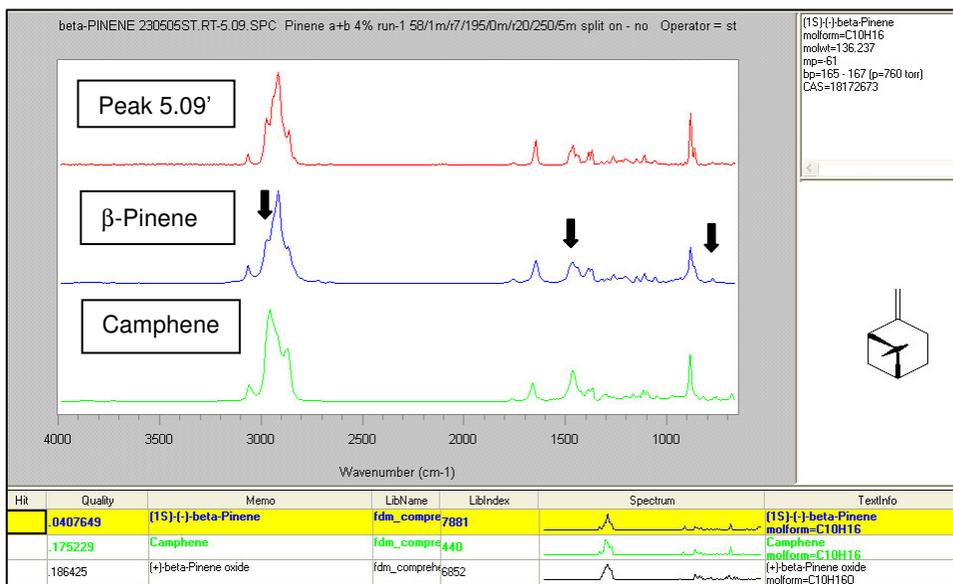
Another key feature of Infrared analysis is that absorption at a certain wavelength is in direct proportion to the amount at hand. Therefore, relative quantities can be determined with confidence, avoiding errors due to disparity in ionization or presence of chromophores.

## Compound Identification using Infrared library searching



Comparing the spectrum for the peak at 4.37 minutes to the IR library gives hits to both  $\alpha$ - &  $\beta$ -pinene. The arrows point to clear features that help make the assignment easy:  $\alpha$ -Pinene !

The spectrum of the peak at 5.09 min yields the top two possibilities from the library of  $\beta$ -Pinene and Camphene, another  $C_{10}H_{16}$  isomer. Examination of the peak shape and relative heights indicates the former.



### Sample Conditions:

Sample: alpha- & beta-Pinene Standards  
 Concentration: 4%  
 Injection: 1  $\mu$ L using split/splitless injector, split 50:1  
 Column: DB5, 20-meter x 0.32-mm ID, 0.25- $\mu$ m film  
 Conditions: Helium carrier, 1 mL/min  
 Temp program: 58 $^{\circ}$  for 1 min, 7 $^{\circ}$ /min up to 195 $^{\circ}$  C, 20 $^{\circ}$ /min up to 250 $^{\circ}$   
 Sample disc: -55 $^{\circ}$  C  
 Injector, transfer line, restrictor tip all at 250 $^{\circ}$  C