IRD 3 Application Note

Unknown Forensic Sample

Introduction

Ever since the advent of the gas chromatograph the chemist has been trying to figure out, "What is that GC peak?" Sample evaluation from a quantitative sense cannot be done accurately without knowing which compound one is looking. Hence the need for smart GC detectors.

With the coupling of the mass spectrometer to the gas chromatograph, the analyst felt that the ultimate GC detector has been found. The thousands of MS's in the world testify to this notion. The MS is smart GC detector; it gives important molecular mass related structural information. Through careful spectral interpretation of the fragment ions, the structure of the original molecule can often be pieced together and the molecular weight can de deduced as well.

However, regardless of how great the power of the mass spectrometer is as a GC detector, it has some weaknesses. These specifically relate to the spatial geometry of the molecule, which is destroyed or masked by the ionization / fragmentation / rearrangement processes of the MS. The IRD 3 from ASAP Analytical helps to overcome these inherent difficulties.

Another smart detector, the IRD 3 utilizes a flow cell that allows one to analyze the intact molecule. This powerful benefit arises because the molecules are freely rotating and isolated from each other in a low energy environment. The IRD's vapor phase spectra are not only molecularly unique, but highly reproducible as well. In the IRD the aspects of a molecule's geometry are kept intact. There are several important areas of structural determination in which the IRD excels.

The sample presented in this application note was submitted to ASAP Analytical and was completely unknown to the customer making the request.

Product Overview

The IRD 3 is designed from the chromatographer's point-of-view and is the only analytical infrared instrument that seamlessly combines the separating power of the Gas Chromatography with the molecular identification of FTIR.

- Dedicated FTIR for use with GC
- Low maintenance and easy to use
- Small footprint
- Software interfaces with GC control software
- Seamless integration with MS

The IRD 3 is the perfect tool for the chromatographer looking to obtain more information about unknown samples. Using a heater light pipe flow cell, the sample is kept in a vapor state while interacting with IR. This allows the molecules to freely rotate in a low energy environment. Keeping the molecular geometry in tack during analysis provides unique and highly reproducible spectra.

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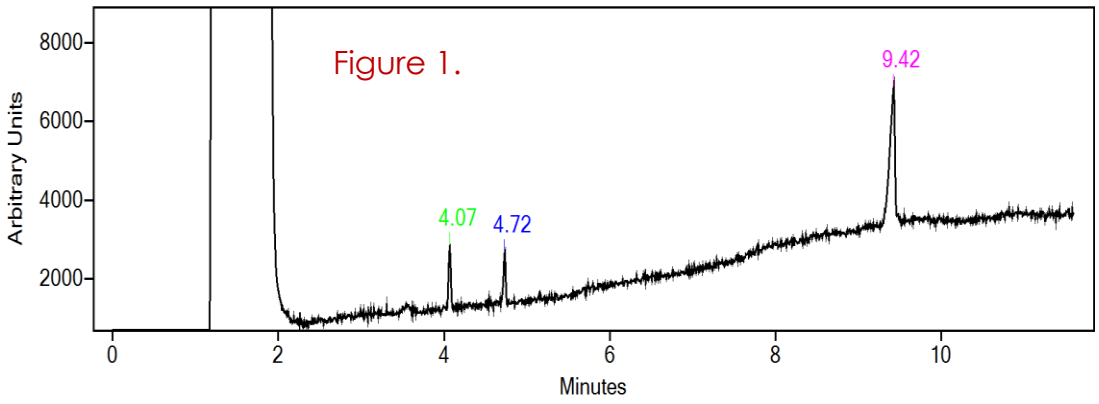
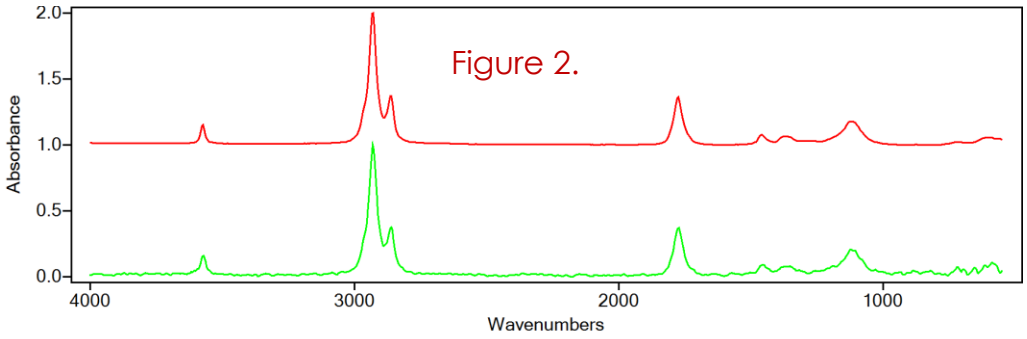
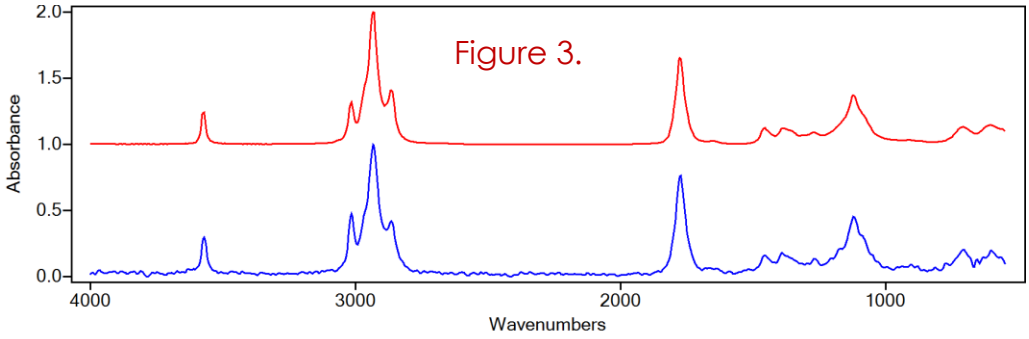
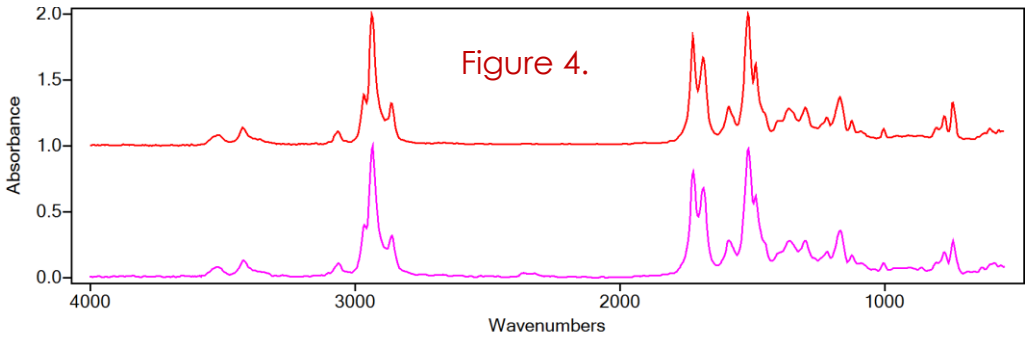
Results

The chromatographic results (Figure 1) showed that three compounds were present. All three chromatographic peaks were then library searched. Peak #1 was identified with a match of 99.3% by the Aldrich vapor phase library as Palmitic Acid (Figure 2). The second peak chromatographic peak was also matched to an entry in the Aldrich vapor phase library with a quality of 99% to Linolenic (Figure 3.). The spectra for the final chromatographic peak was matched with an entry in the ASAP IRD Users Library. The spectra had a 99.5% match to AB-Chminaca(Figure 4), a synthetic cannabinoid.









Conclusion

The IRD 3 is an excellent choice when a sample of unknown origin or composition needs to be identified. The IRD 3 uses a heater light pipe flow cell, the sample is kept in a vapor state while interacting with IR. This allows the molecules to freely rotate in a low energy environment. Keeping the molecular geometry in tack during analysis provides a unique and highly reproducible spectra.

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