IRD 3 Application Note

Differentiation of Ethylone, Eutylone, Pentylone and Butylone

Introduction

Novel designer drugs can be difficult to analyze by GC-MS. With the addition of vapor phase GC-IRD the differentiation of these compounds can be accomplished with greater ease. Vapor phase GC-IRD offers fast analysis and has the same sample preparation as GC-MS. An optional transferline allows an MS detector to be seamlessly added to the GC-IRD so that both IR and MS data can be obtained from a single GC injection. In combination the GC-IR-MS represents the most powerful analytical tool for the identification of unknowns and isomeric compounds.

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.

Results

As shown in Figure 1, the library search results for all four compounds are not conclusive. Figures 2 and 3 show the spectra in stacked mode and overlay mode and confirm how similar the spectra are for these four compounds. Since library search results cannot be used solely to determine the exact identity of these compounds one must look to other data analysis tools. Figure 4 shows a zoomed in view of the 3100-2800 wavenumber region. To help with the identification just this region of the spectra was searched. Highlighting only the region that has differences can assist in better quality matches. If the results of a region search are inconclusive the analyst can also turn to retention time and MS results.

Figure 1.

Sample Name	#1 hit	#2 hit	#3 hit	#4 hit
Eutylone	99.7% Eutylone	99.4% Pentylone	99.2% Butylone	98.9% Ethylone
Pentylone	99.7% Pentylone	99.2% Eutylone	98.9% Butylone	98.2% Ethylone
Ethylone	98.6% Ethylone	97.5% Eutylone	97.5% Butylone	97.4% Pentylone
Butylone	99.6% Butylone	99.5% Pentylone	99.4% Eutylone	98.9% Ethylone

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Figure 2.

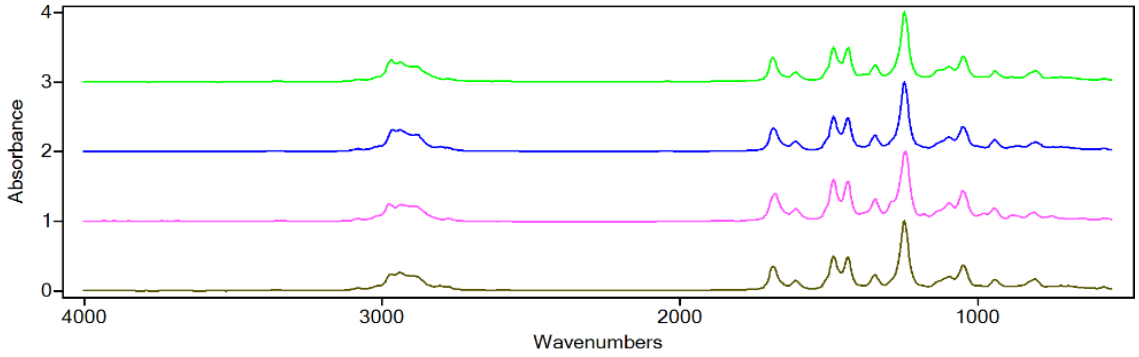


Figure 3.

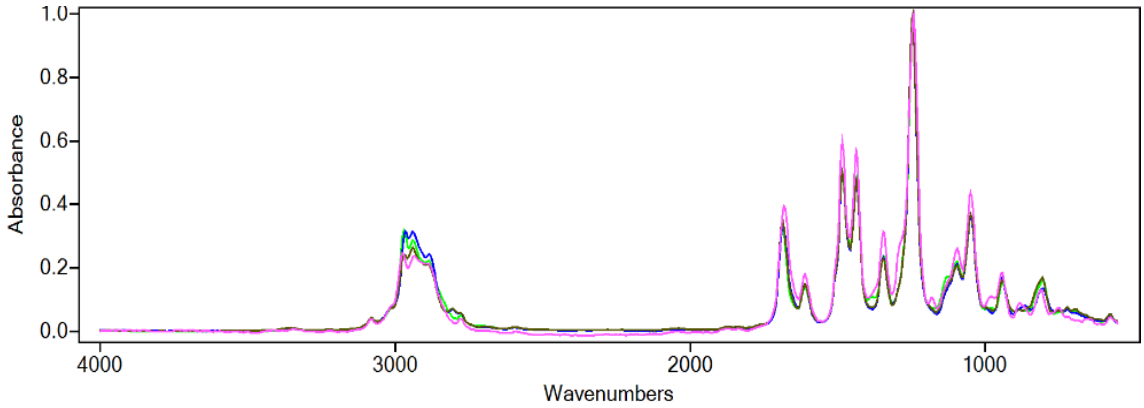
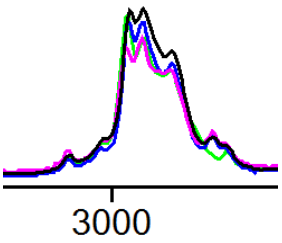


Figure 4.



Conclusion

The IRD 3 is the perfect tool to assist the chromatographer in identification of similar compounds. 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.