

## IRD 3 Application Brief

### PNA Ring Junctions

#### Introduction

While the mass spectrometer produces powerful structural information based on molecular fragmentation, often including molecular weight data, MS can be weak differentiating polynuclear aromatic hydrocarbons (PNA) ring bonding. Conversely, the infrared spectrometer is strong in these areas.

This note highlights the power of the ASAP Analytical IRD 3 to aid in the distinguishing of a pair of polynuclear aromatic hydrocarbons with nearly identical MS spectra. While this example is chosen from the area of industrial chemistry, knowledge of PNA ring bonding has broad applicability in all area where structural identification is important.

#### 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.



#### Parameters and Results

A high confidence determination of these two PNA compounds was achieved using the Aldrich Vapor Phase Library (099-1908). Searches were conducted for both fluoranthene and pyrene and the results show high quality index matches for both compounds.

#### Conclusion

The GC-IRD has been shown to be useful in the differentiation of similar polynuclear aromatic hydrocarbons, specifically in this example of fluoranthene and pyrene.

