Introduction

Bath salts are an emerging class of “recreational” drugs of abuse that contain one or more synthetic chemicals related to cathinone. Cathinone is an amphetamine-like stimulant naturally found in Khat, a flowering plant native to the Horn of Africa. Dangerous health effects and extreme intoxication have made these bath salts a health and safety concern. Users of synthetic cathinones experience various effects ranging from euphoria to paranoia and even death. Marketed as bath salts in an attempt to mask their true identity, they typically come in white or brown crystalline powder and are labeled “Not for Human Consumption”.

Synthetic cathinones present a significant challenge for the modern forensic lab. Although new laws have been passed to prohibit similar “analogues” to previously banned synthetic cathinones, manufactures have responded by creating new drugs that differ enough to evade present legal restrictions. The compounds presented in this application note are an excellent example. This “cat and mouse” game makes the job of the forensic chemist extremely difficult. Identifying with certainty the exact compound or differentiating between two very similar positional isomers can be a significant challenge. The IRD 3 from ASAP Analytical can complement other laboratory detectors and techniques to ensure that all compounds are identified with the highest level of certainty.

This application note shows an example of two positional isomers, 2,3 and 3,4-MDPV, that produce identical mass spectra. However, their IR spectra collected on the IRD 3 are significantly different, allowing proper identification of each isomer.

Product Overview

The IRD 3 is designed from the chromatographer’s point-of-view and is unique in that it was designed to be used directly with a Gas Chromatograph (GC), and not just as a lab top FTIR. The IRD-3 seamlessly integrates the separating power of the GC with the molecular identification of an FTIR.

The IRD 3 is the perfect tool for the chromatographer looking to obtain more information about unknown samples. Using a heated light pipe flow cell, the sample is kept in the vapor state while interacting within the IR band width. Keeping the molecular geometry intact during analysis provides unique and highly reproducible spectra.

Results

Figure 1 shows the EI-MS spectra for 2,3 and 3,4-MDPV and confirms the spectra are essentially identical. The figure also includes the structure of each molecule and the region of the IR spectra from 1500-1000 wavenumbers. Much of the IR spectra are identical but the region shown has distinct differences that are highly reproducible. The spectra for 2,3 has a single peak at 1446 that corresponds to a doublet in the 3,4 spectra. The reverse is true for the 3,4 spectra, where a large single peak is present at 1246 and a doublet is present at this location on the 2,3 spectra.
Conclusion

This example illustrates the tremendous power of the IRD to distinguish between compounds which are very similar structurally. It also points out the excellent complementary information that the IRD and MSD provide. The combination of these two detectors provides exceptional capability for qualitative analysis at a very high confidence level. When using them in series with a GC, you have the ability to confirm identity of compounds by two techniques and also to use the IRD to differentiate between isomers.