

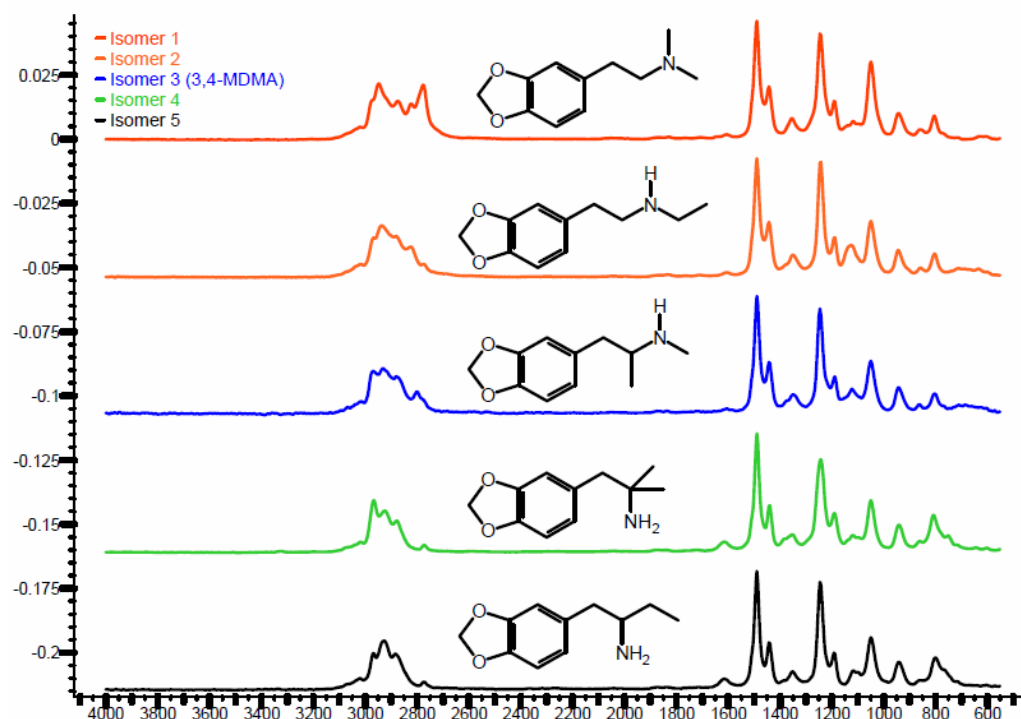
Infrared Detector

REMOVING ANY DOUBT FROM THE FORENSIC IDENTIFICATION OF 3,4-MDMA BY INCLUDING GC-IRD

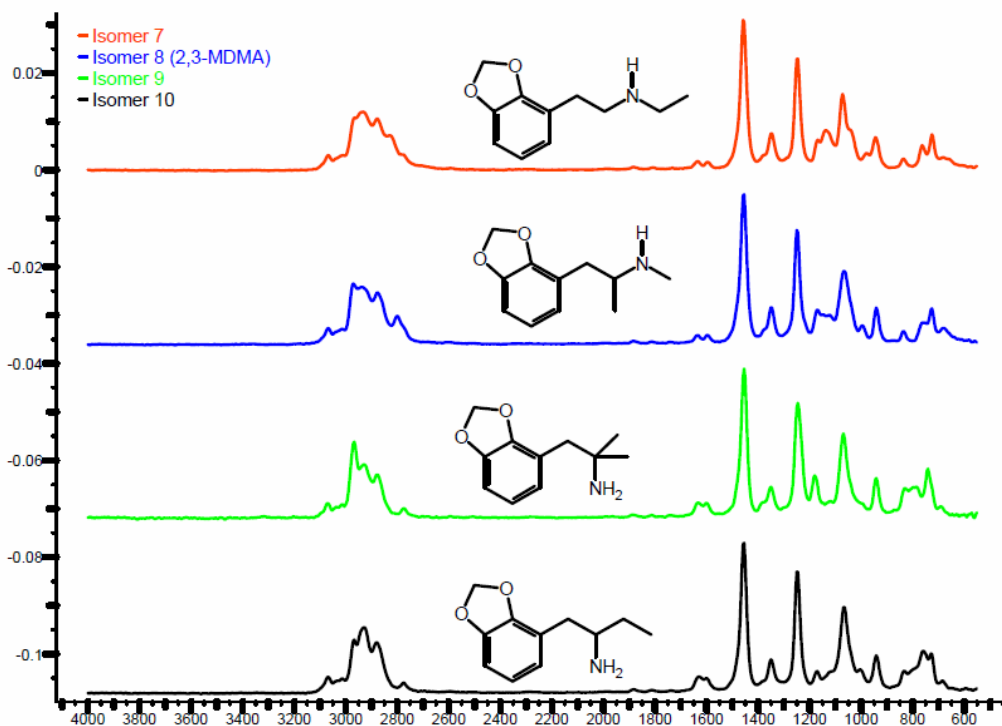
Isomeric forms of synthetic drugs of abuse, particularly phenethylamines, can be problematic by conventional GC.MS methods. Another of these phenethylamines, 3,4-methylenedioxymethamphetamine (3,4-MDMA), more commonly known as "Ecstasy", has been the subject of extensive research in Forensic Analytical Chemistry. Of particular significance is that 3,4-MDMA and its many related isomers and isobaric compounds frequently yield minimal mass fragmentation detail, and in some cases the ambiguity of the mass spectral data obtained places the analyst in a tenuous, unenviable position to provide identification "beyond a reasonable doubt". GC.IRD data from 3,4-MDMA and a series of its isomers and isobaric compounds has now been collected, and has proven to provide the analyst additional data to complement the GC.MS data in asserting the identification of these types of compounds. Finally, new and advanced data analysis software applying principal components analysis to the MS and IRD data will be presented in an effort to understand the underlying issues.

" This approach (MS) can be dangerous because different molecules can have indistinguishable mass spectra.... The structures of the isomers varies in such a way that the corresponding fragments have the same mass-charge ratio in each spectrum. The spectra are therefore, essentially equivalent, with some minor variation in peak intensities.... No absolute "fingerprint", then, can be established..."

*Comments on the analysis of the 10 Isomers of "ecstasy" by GC/MSD.
Filmore, David, Today's Chemist at Work, Feb. 2001, 27-32.*



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Summary

- GC Retention Time differences small.
- Differentiation by MS frequently relies on very minor peaks.
- Ambiguities noted.
- MS Data can be difficult for layman to understand and accept conclusion.
- GC.IRD results unique.
- Differentiation by IRD sensible.
- Spectra/structure correlations observed.
- IRD Data and a simple explanation sufficient for layman to understand, accept and believe conclusion.
- Value of IRD in Isomer differentiation is unsurpassed
- IRD provides a simple solution
- Product is a complementary technique to the GC-MS, not an alternative