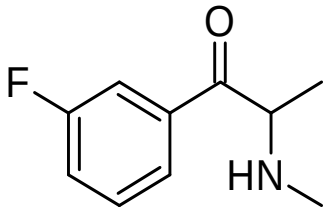


DiscovIR-GC®

Deposition and Detection System

Application Note 40

Designer Drug Identification: Fluoromethcathinone Isomers Identifed with the DiscovIR-GC Instrument

Forensic drug laboratories have become the first line of defense in the fight against new and dangerous designer drugs. Many of these substances are designed with slight chemical modifications to a parent structure; making the unequivocal identification of particular compounds a challenging problem. Archer[1] recently described the analysis of 3' fluoromethcathinone found in a product sold as a plant feeder. He compared the analytical data for three isomers of fluoromethcathinone (2', 3', and 4' fluoro) and concluded that all three isomers contained no significant differences in their mass spectra. His results showed that the GC elution times were very similar to each other but the fluoromethcathinones (FMC) did reveal useful differences for identification using Infrared Spectroscopy. This application note details the analysis of 3'-FMC and 4'-FMC using the DiscovIR-GC® instrument. The DiscovIR-GC uses a GC to separate complex mixtures into separate components deposited upon a rotating infrared transparent disc. An Infrared spectrum is then collected of the individually separated GC components.

Figure 1 below shows two isomers of fluoromethcathinone which depicts the similarity in structure between these drugs. Examination of Figure 2 (Page 2) shows that these compounds can be easily differentiated via Infrared spectroscopy. The differences are accentuated in the fingerprint region shown in Figure 3 (Page 3) where the instrument software allows overlays of the spectra to clearly identify both isomers. The spectra are rich in data as even those peaks which predominate in each spectrum reveal significant wavenumber differences (see the range from 1700-1600 cm^{-1}).

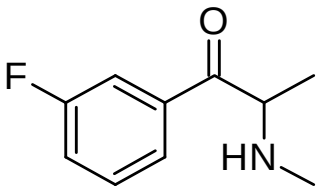
The mass spectra for these two isomers shown in Figure 4 (Page 3) demonstrate the comparative value of IR versus MS. Besides the base peak at 58 m/z, the mass spectra show little data above 10% abundance. In addition, the mass spectra of these isomers are essentially identical, making identification by GC/MS dependent on subtle differences in retention time (see table below for retention time data).

	HP-5 MS Column (30m)	DB-1 MS Column (30m)
3'-FMC Retention Time	**9.23 min.[1]**	**5.69 min.**
4'-FMC Retention Time	**9.27 min.[1]**	**5.74 min.**
	Hold 80°C 4 min. Ramp to 280°C @ 20°C/min.	Hold 100°C 1 min. Ramp to 300°C @ 12°C/min.

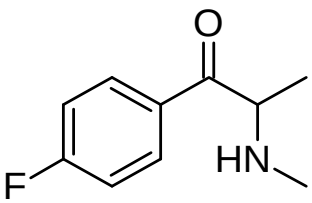
The DiscovIR-GC instrument provides for the efficient separation and rapid identification of complex mixtures of closely related compounds. As shown here, even very similar isomers can be uniquely identified by this technique. As the nature of drug analysis changes and new challenges become commonplace, the forensic drug chemist will need additional tools to permit identification of drugs that may differ only slightly in structure and reveal very similar features in an MS analysis. The DiscovIR-GC system is an effective tool in the identification of closely related compounds and offers an excellent alternative or complementary technique to those analyses routinely used in the forensic laboratory.

[1]Archer, R.P, Forensic Science International 185 (2009) 10–20

Figure 1



3' -fluoromethcathinone



4' -fluoromethcathinone

Standards provided by Cayman Chemical

Spectra Analysis

The Leader in GC-IR and LC-IR Instrumentation

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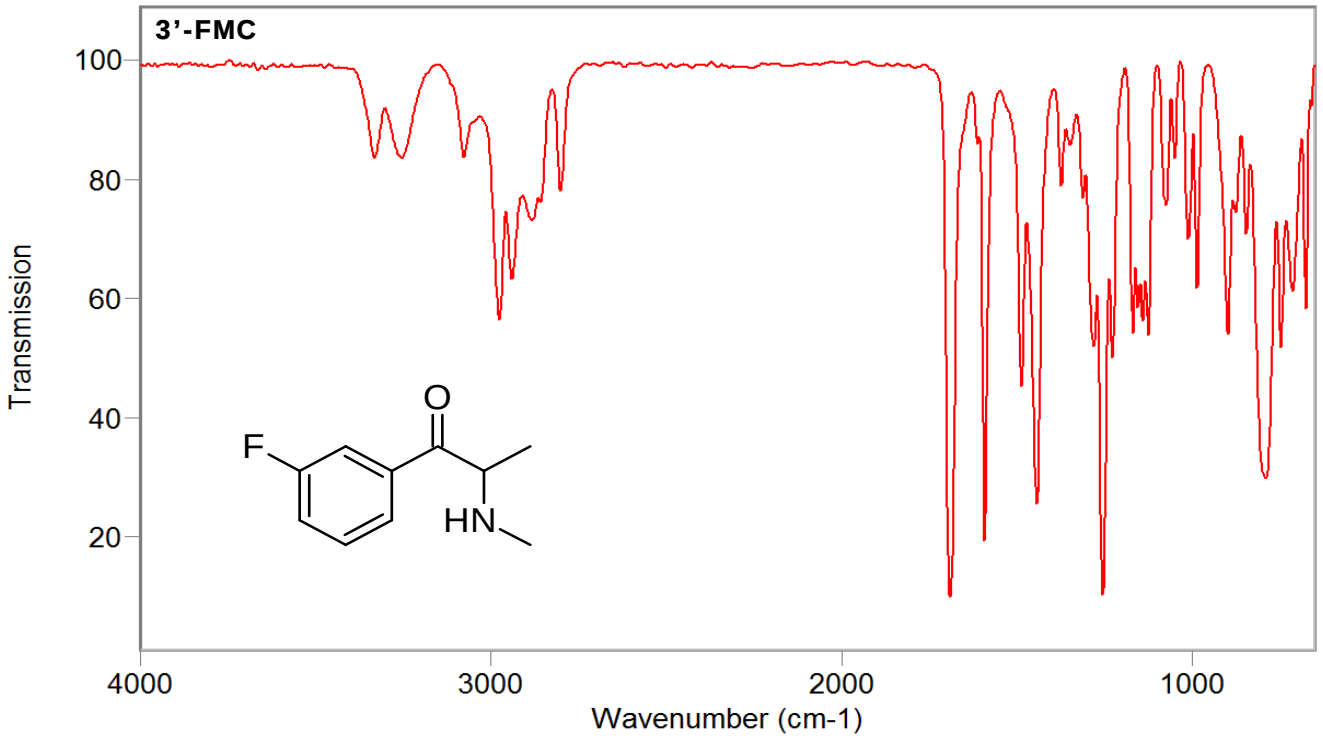
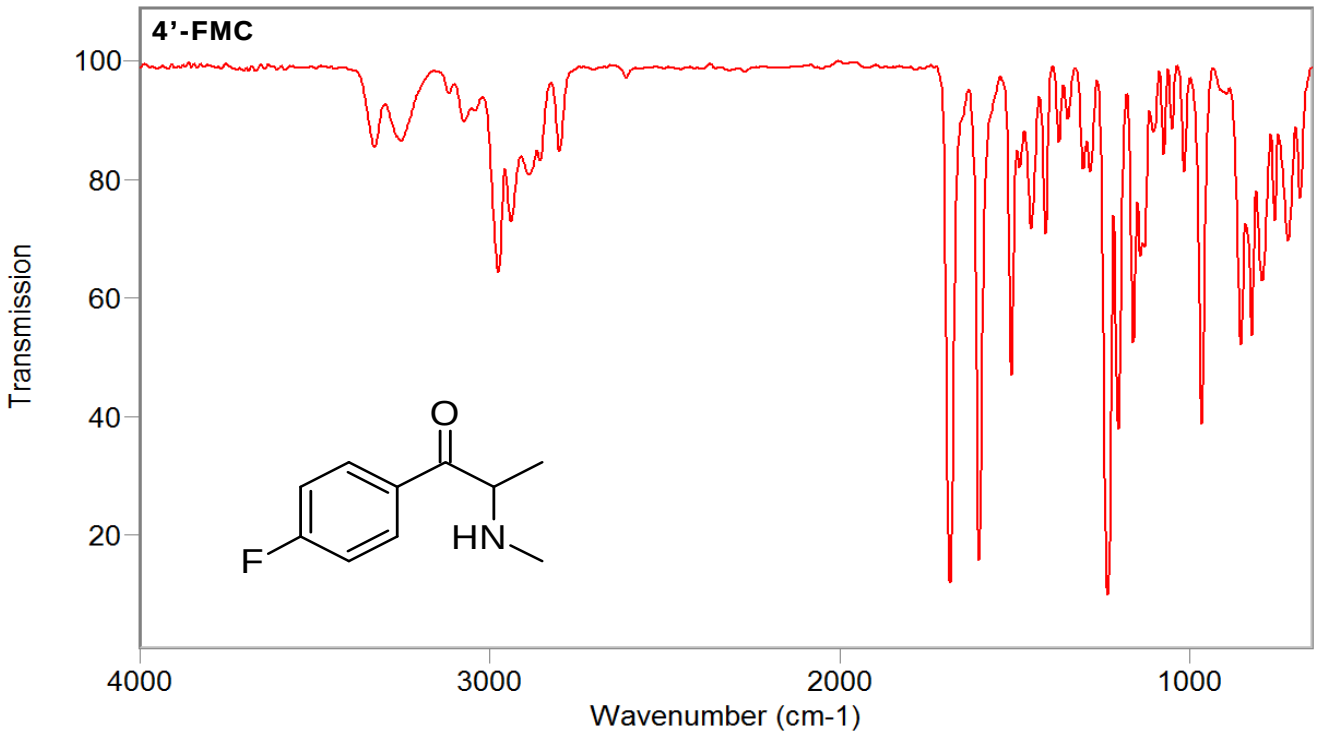
Figure 2

DiscovIR-GC® Infrared Spectra





Spectra provided by Canada Border Services

Figure 3

Fluoromethcathinone Isomers at 4 cm^{-1} Resolution

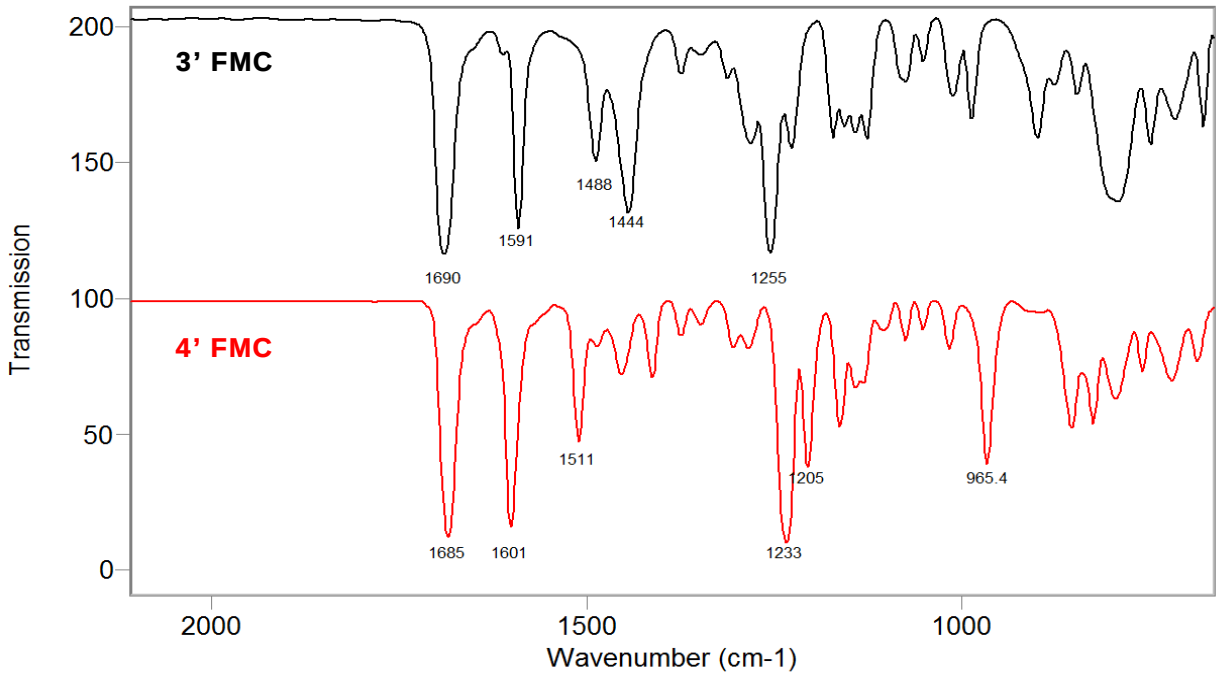
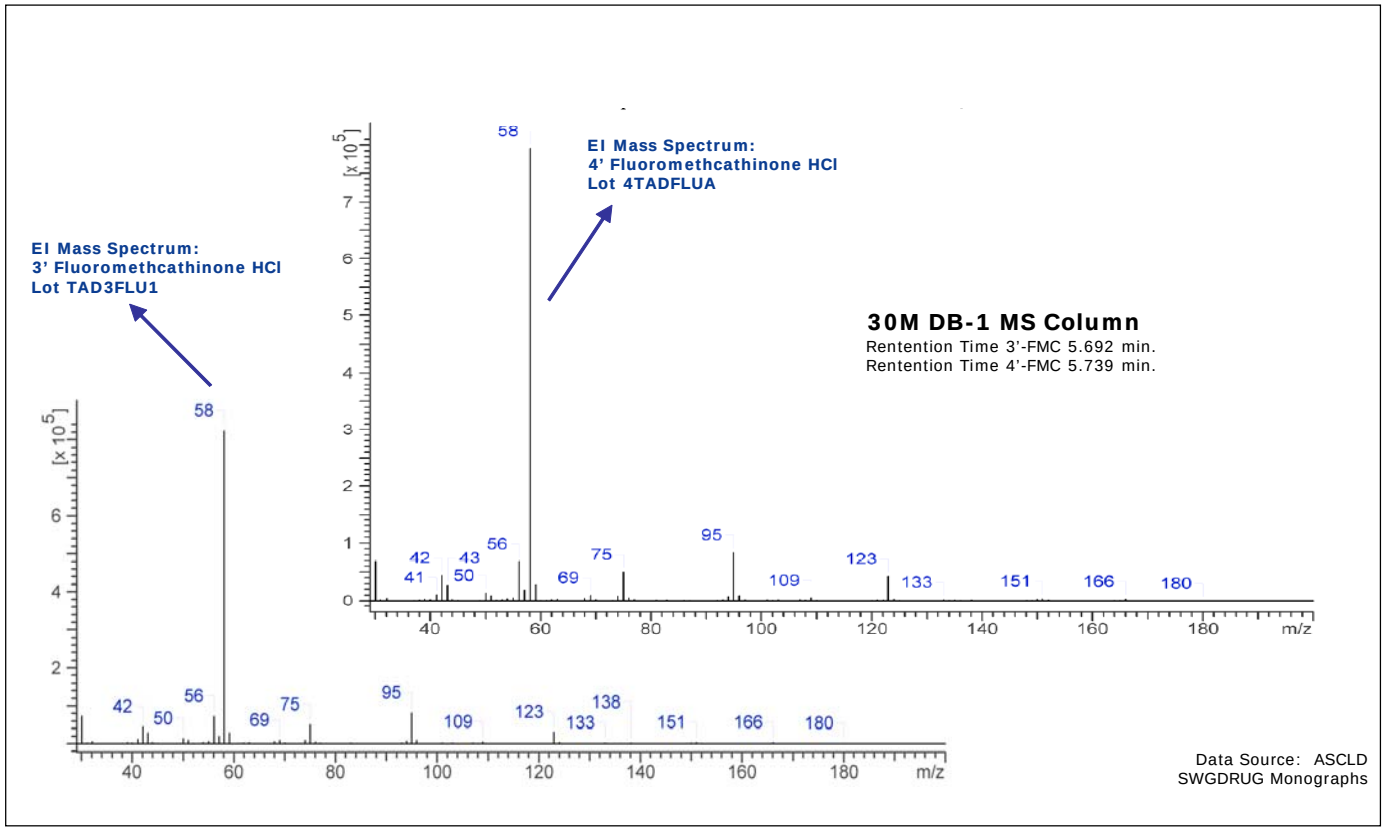


Figure 4

GC-MS of 3'-FMC and 4'-FMC



DiscovIR-GC® Specifications

Detection Method	Built-In FTIR
IR Detection	0.1 x 0.1 mm MCT
IR Range	4000 - 650 Wavenumbers
Resolution	4 or 8 cm^{-1}
Data Collection	Real Time w/ Post-Run Rescan
Spectrum Type	Transmittance
Disc Capacity	40 Hours
Disc Temperature Control	-70 to +50°C
Unattended Operation	8 hours (LN_2), Auto-Sampler Compatible
Program	Standard Desktop Computer w/Microsoft Windows
Spectroscopy Package	Thermo Galactic Grams™
Standard Features	Real Time and Post-Run Data Collect Chromatographic / Spectral Workup Band Chromatograms, Chemical Class Ratio Chromatograms, Trends Alignment and Tuning Tools Library Search Software Included
Flow Rates	0.1 to 5 mL/min.
Sensitivity	Pico Gram Range
Gradients	N/A
Chromatograph	Any GC (supplied by user)

Spectra Analysis

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