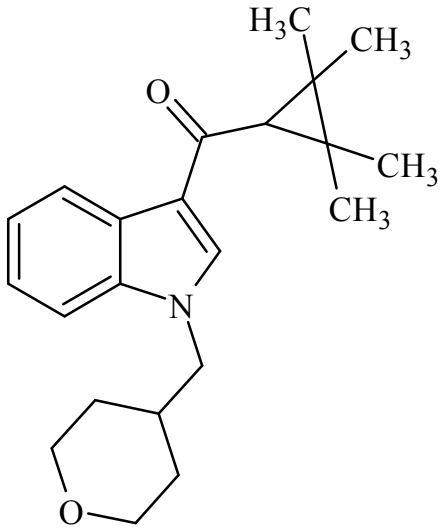
# A-834,735

*The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.*



## *1. GENERAL INFORMATION*

***IUPAC Name:*** [1-(tetrahydro-2*H*-pyran-4-methyl)-1*H*-indol-3-yl]-(2,2,3,3-tetramethylcyclopropyl)methanone

***CAS#:*** 895155-57-4

***Synonyms:*** [1-(tetrahydropyran-4-ylmethyl)-1*H*-indol-3-yl]-(2,2,3,3-tetramethylcyclopropyl)methanone

***Source:*** DEA Reference Material Collection

***Appearance:*** White powder

***$UV_{max}$(nm):*** Not Determined

## *2. CHEMICAL AND PHYSICAL DATA*

### 2.1 CHEMICAL DATA

| Form | Chemical Formula | Molecular Weight | Melting Point (°C) |
|---|---|---|---|
| Base | $C_{22}H_{29}NO_2$ | 339 | 137.9 |

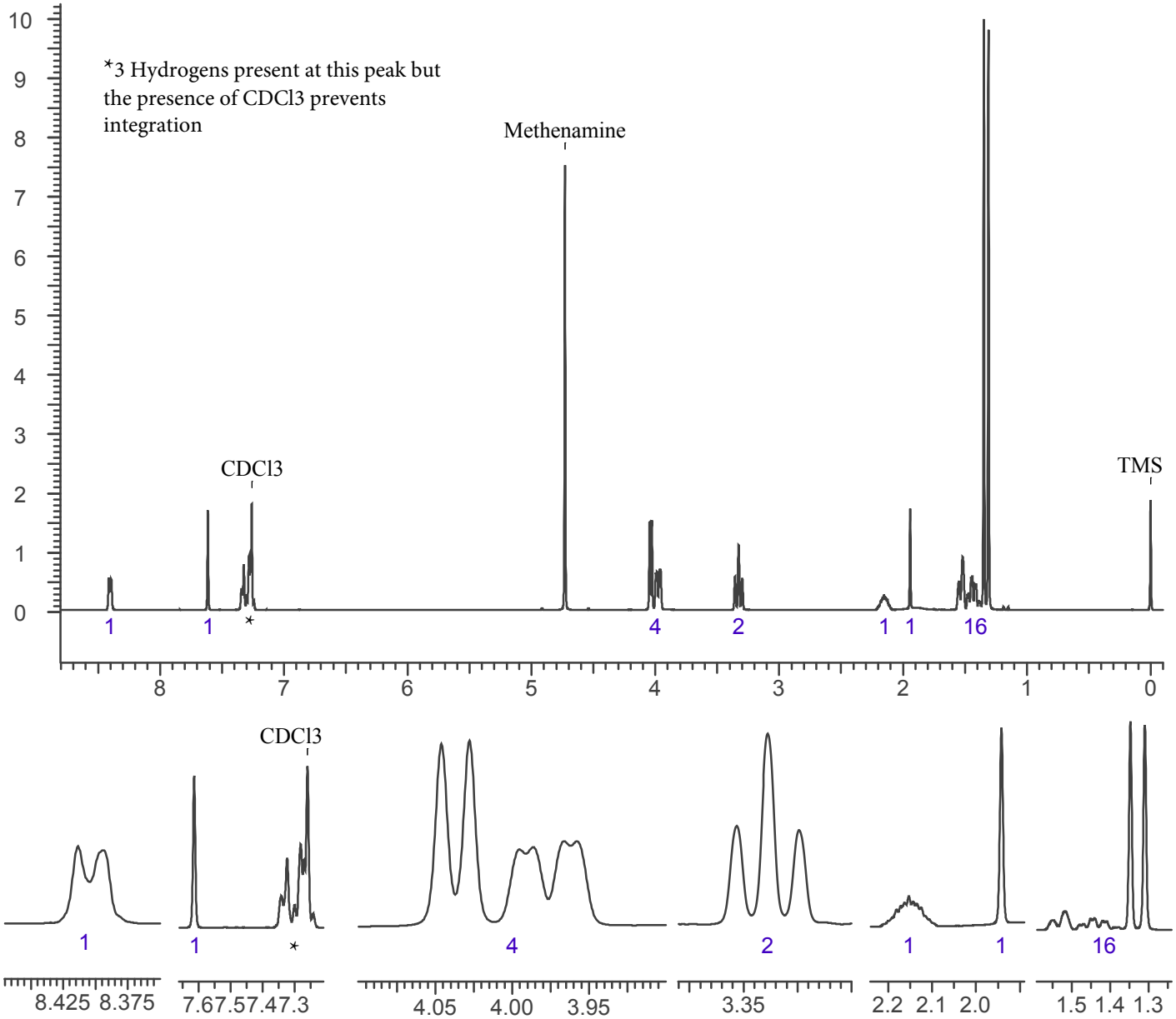
## *3. QUALITATIVE DATA*

### 3.1 NUCLEAR MAGNETIC RESONANCE

*Sample Preparation:* Dilute analyte to ~16 mg/mL in $CDCl_3$ containing TMS for 0 ppm reference and methenamine as quantitative internal standard.

***Instrument:*** 400 MHz NMR spectrometer
***Parameters:*** Spectral width: at least containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds

$^1$H NMR: A-834,735 Lot RM-131001-05, $CDCl_3$, 400MHz

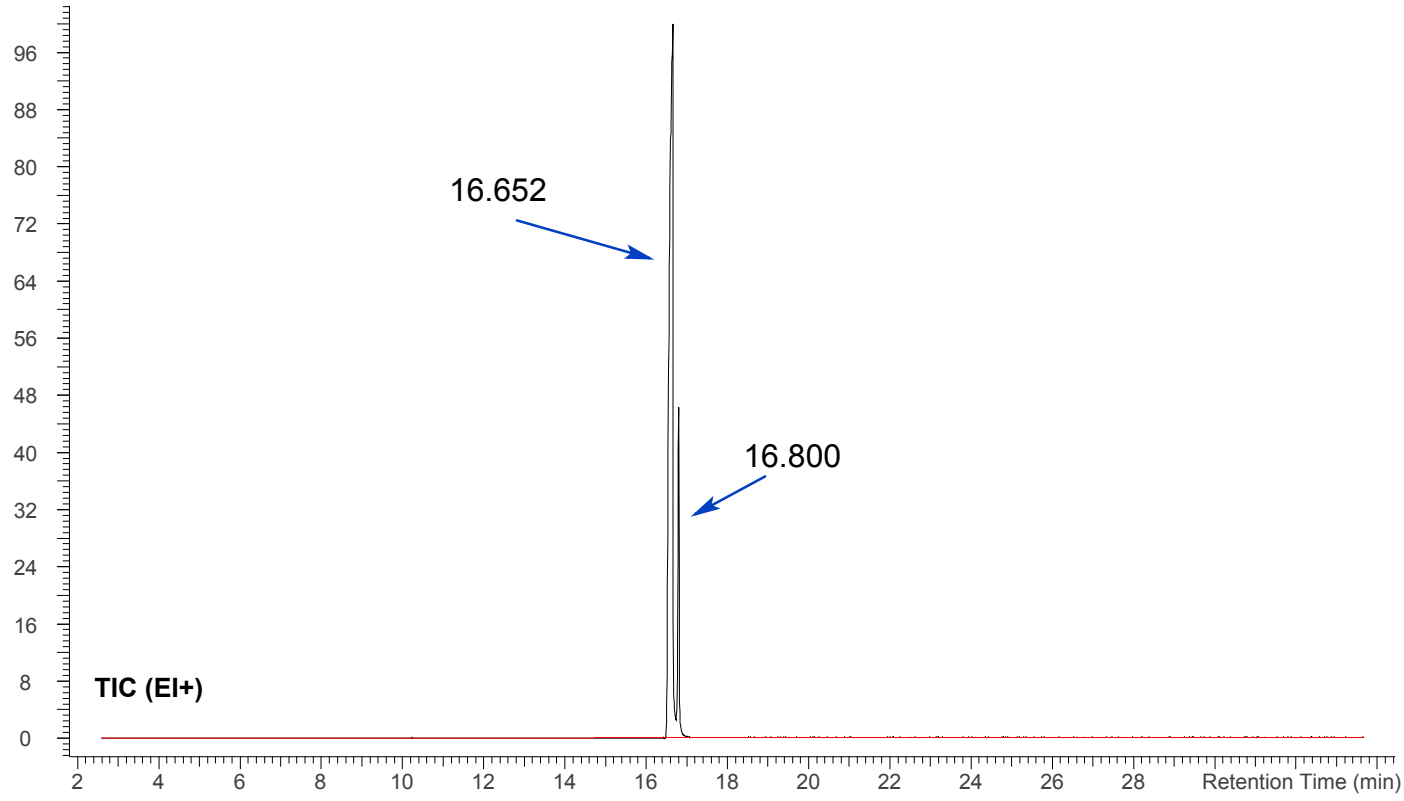


## 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

*Sample Preparation:* Dilute analyte ~4 mg/mL in methanol

| | |
|---|---|
| ***Instrument:*** | Agilent gas chromatograph operated in split mode with MS detector |
| ***Column:*** | DB-1 MS (or equivalent); 30m x 0.25 mm x 0.25 µm |
| ***Carrier Gas:*** | Helium at 1 mL/min |
| ***Temperatures:*** | Injector: 280°C |
| | MSD transfer line: 280°C |
| | MS Source: 230°C |
| | MS Quad: 150°C |
| | Oven program: |
| | 1) 100°C initial temperature for 1.0 min |
| | 2) Ramp to 300°C at 12 °C/min |
| | 3) Hold final temperature for 16.0 min |
| ***Injection Parameters:*** | Split Ratio = 25:1, 1 µL injected |
| ***MS Parameters:*** | Mass scan range: 34-550 amu |
| | Threshold: 100 |
| | Tunefile: stune.u |
| | Acquisitionmode: scan |
| ***Retention Time:*** | A-834,735peakat16.652min.,Rearrangementpeakat16.800min. |

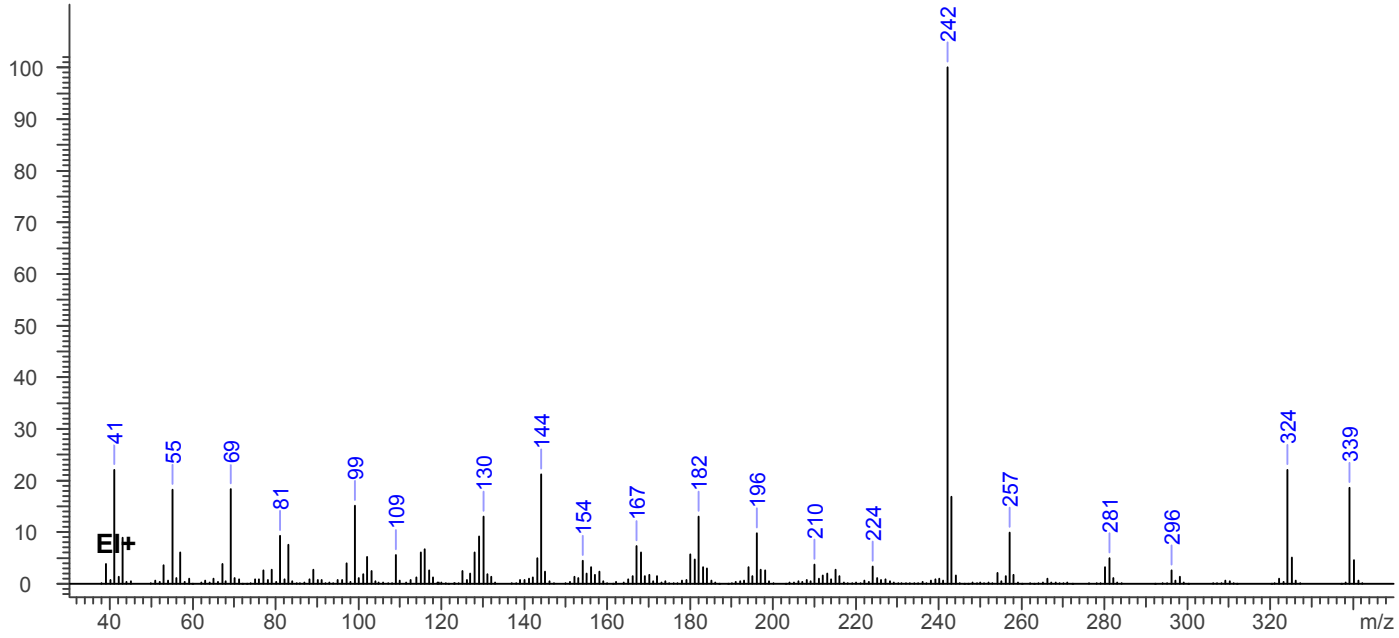
GC/MS TIC: A-834,735 Lot RM-131001-05



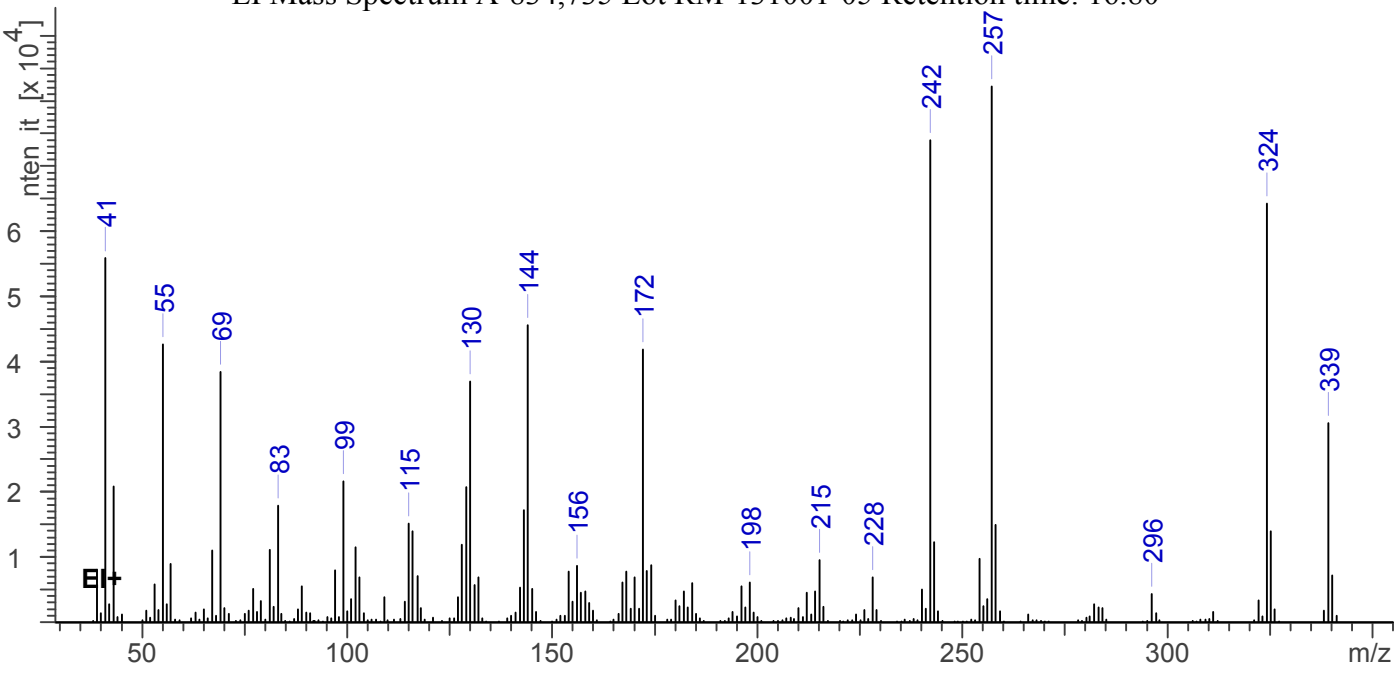
**GC/MS Analytical Observation:**

The GC/MS TIC for A834,735 shows two peaks with similar mass spectra. The major peak, having a retention time of 16.652 minutes is A-834,735 while the other peak with a retention time of 16.800 minutes, is a thermally induced rearrangement product of A-834,735. This rearrangement product is an artifact induced by the high temperature of the GC injection port.

GC/MS TIC: A-834,735 Lot RM-131001-05




EI Mass Spectrum A-834,735 Lot RM-131001-05 Retention time: 16.80

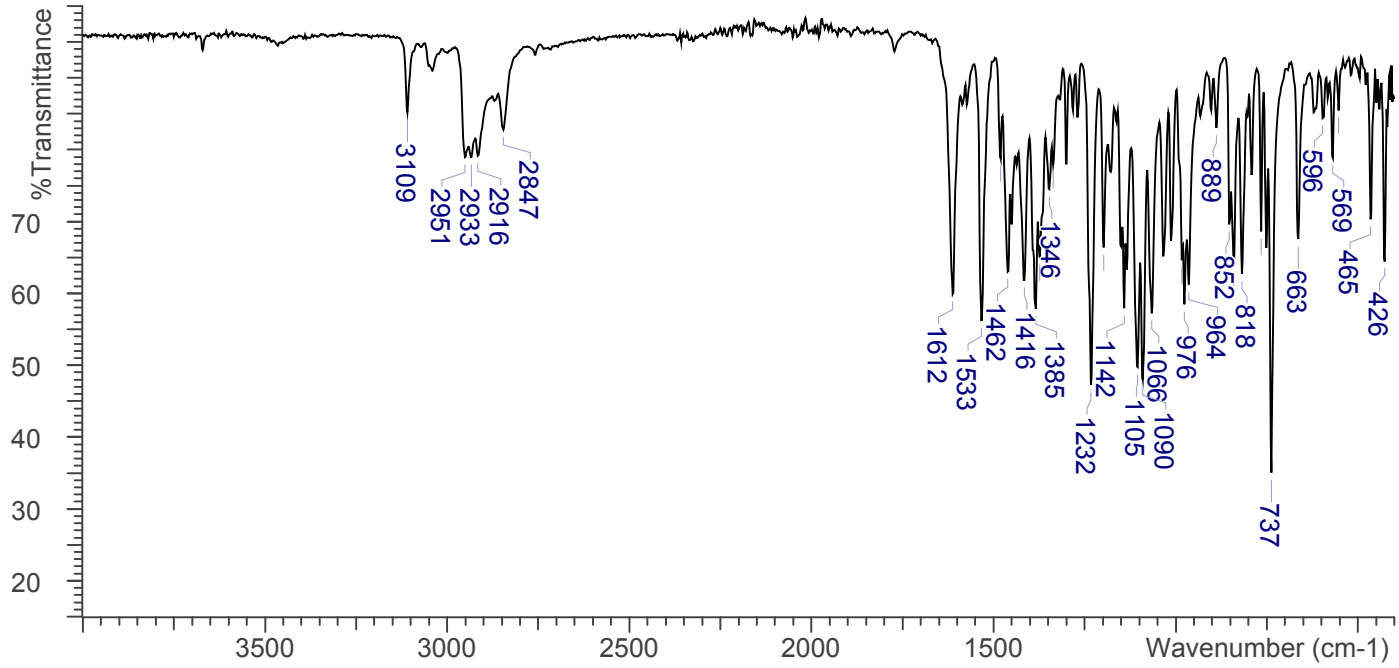


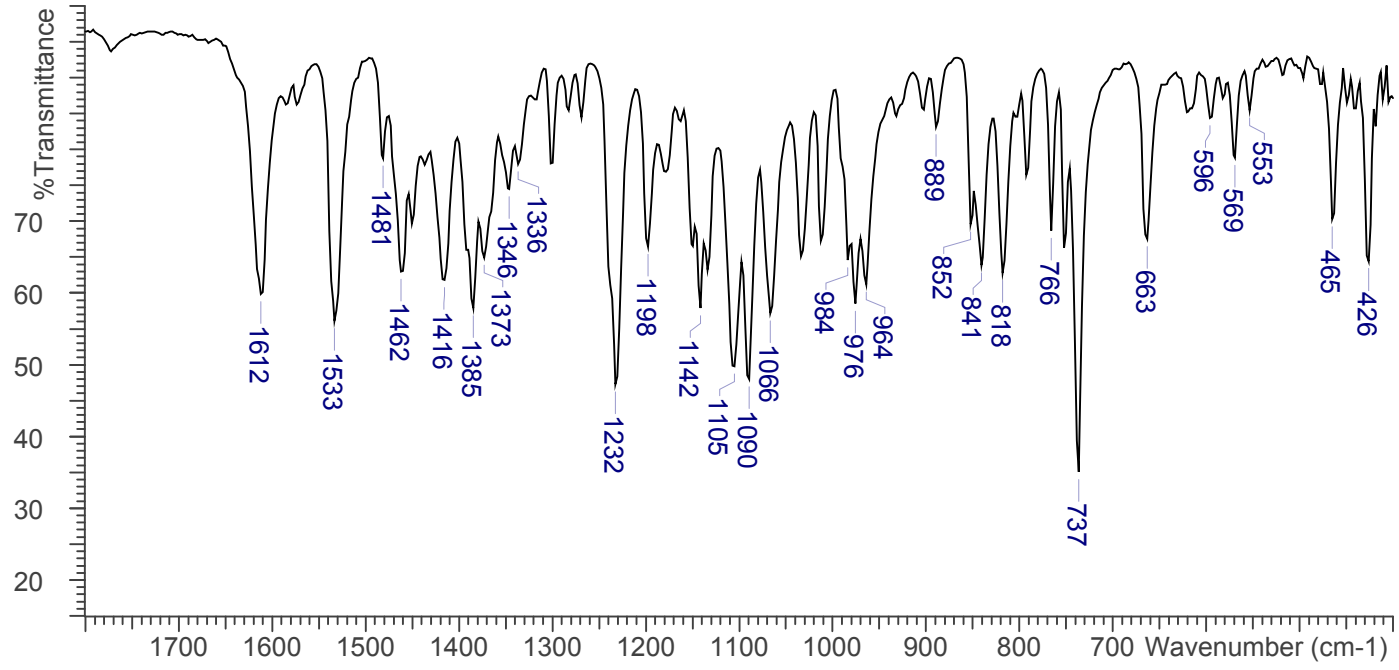
### 3.3 INFRARED SPECTROSCOPY (FTIR)

**Insrument:** FTIR with diamond ATR attachment (3 bounce)

**Scan Parameters:**
Number of scans: 32
Number of background scans: 32
Resolution: 4 $cm^{-1}$
Sample gain: 8
Aperture: 150

FTIR ATR (Diamond, 3 Bounce) A-834,735 Lot # RM-131001-05



## *4. ADDITIONAL RESOURCES*

***Wikipedia***

***Forendex***

Zuba, D.; Geppert, B.; Sekula, K.; Zaba, C.; [1-(Tetrahydropyran-4-ylmethyl)-1*H*-indol-3-yl]-(2,2,3,3-tetramethylcyclopropyl)methanone: a new synthetic cannabinoid identified on the drug market. Forensic Toxicol (2013) 31: 281-291.

Uchiyama, N. et al. Identification of two new-type designer drugs, piperazine derivative MT-45 (IC-6) and synthetic peptide Noopept (GVS-111), with synthetic cannabinoid A-834735, cathinone derivative 4-methoxy-α- PVP, and phenethylamine derivative 4-methylbuphedrine from illegal products. Forensic Toxicol. DOI 10.1007/s11419-013-0194-5.