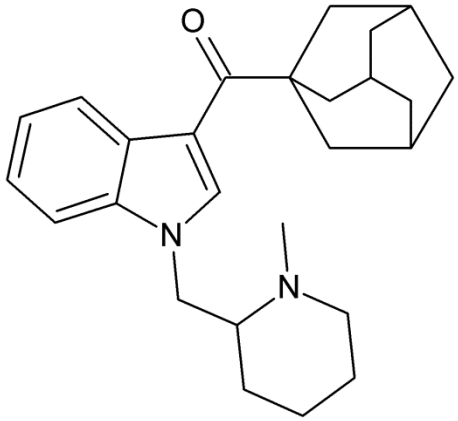



## *1. GENERAL INFORMATION*

***IUPAC Name:*** {1-[1-methylpiperidin-2-yl]-1H-indol-3-yl}(tricyclo[3.3.1.1$^{3,7}$]dec-1-yl)methanone

***CFR:*** Not Scheduled (as of 2/2013)

***CAS #:*** 335160-66-2

***Synonyms:*** 1-[(N-methylpiperidin-2-yl)methyl]-3-(adamant-1-oyl)indole, Adamantan-1-yl{1-[(1-methyl-2-piperidinyl)methyl]-1*H*-indol-3-yl}methanone

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

***Appearance:*** White powder

***Kovat's Index:*** Pending

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

## *2. CHEMICAL AND PHYSICAL DATA*

### 2.1 CHEMICAL DATA

| Form | Chemical Formula | Molecular Weight | Melting Point (°C) |
|---|---|---|---|
| Base | $C_{26}H_{34}N_2O$ | 390 | 143.1 |

## *3. ADDITIONAL RESOURCES*

Forendex

Wikipedia

## *4. QUALITATIVE DATA*

### 4.1 NUCLEAR MAGNETIC RESONANCE

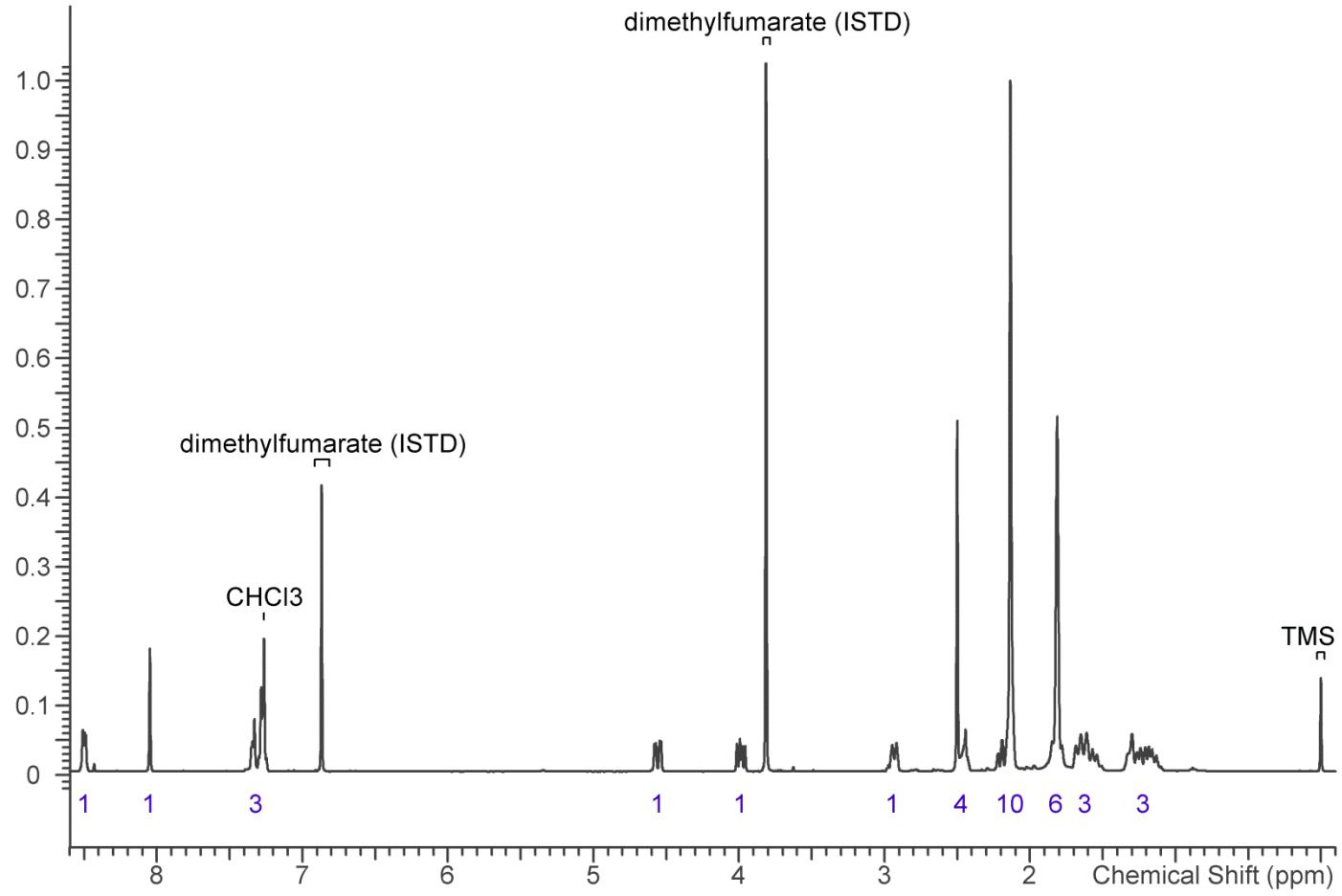
***Method NMR $CDCl_3$***

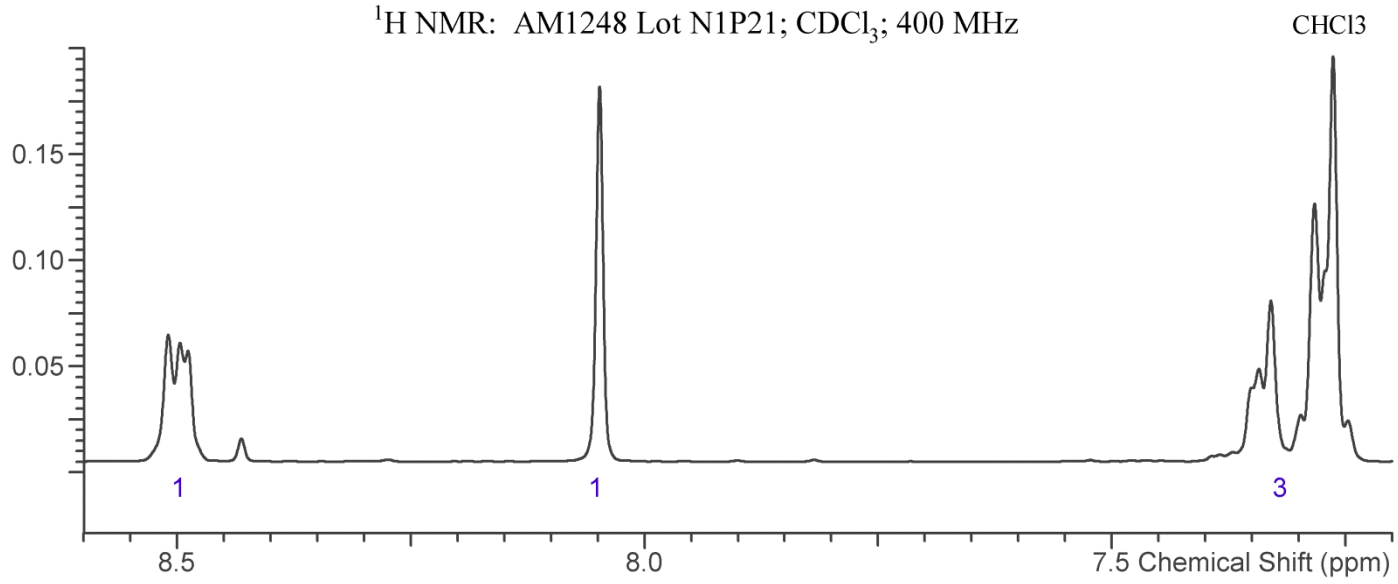
*Sample Preparation:* Dilute analyte to ~10 mg/mL in deuterochloroform ($CDCl_3$) containing TMS for 0 ppm reference and dimethylfumarate as quantitative internal standard.

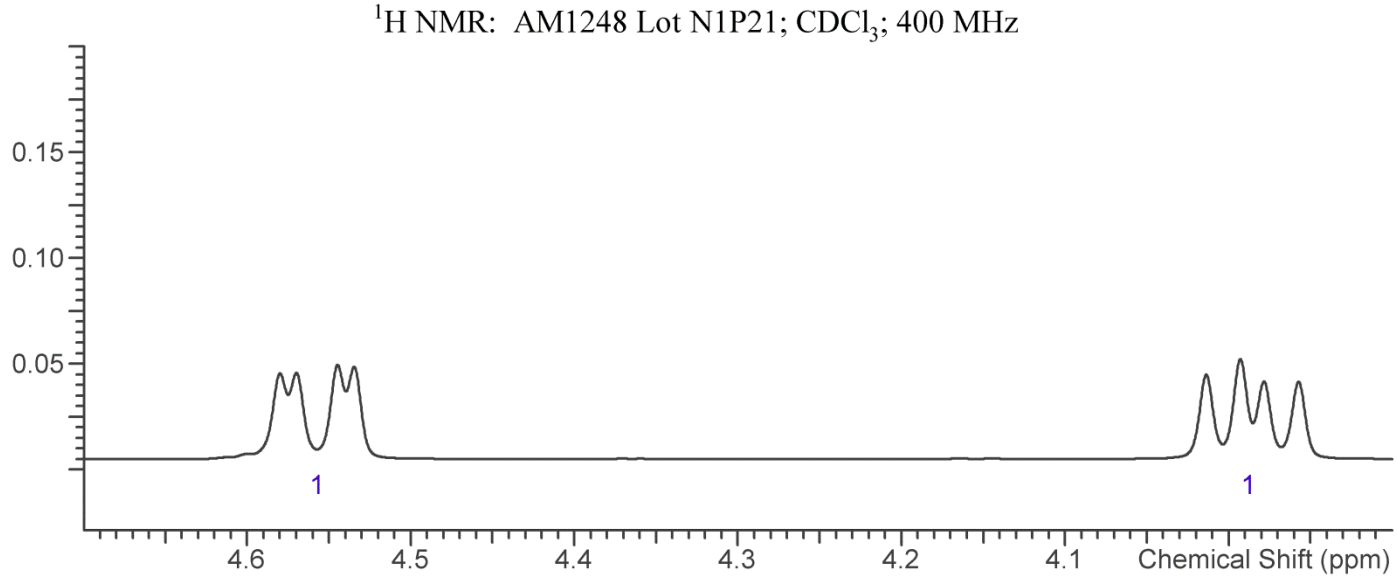
***Instrument:*** Varian Mercury 400 MHz NMR spectrometer with proton detection probe

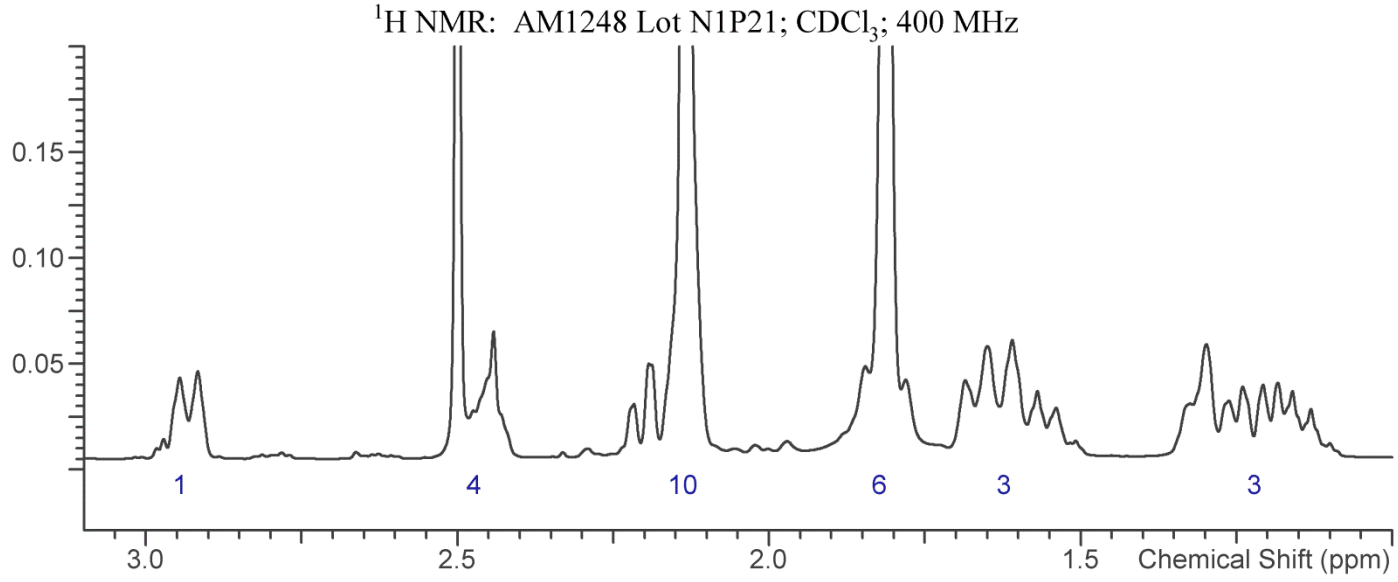
***Parameters:***
Spectral width: at least containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds
Number of scans (NT): 8
Number of steady state scans: 0
Oversampling: 4 or more
Shimming: automatic gradient shimming of Z1-4 shims
Phasing, Drift Correction: automatic or manual

$^1$H NMR: AM1248 Lot N1P21; $CDCl_3$; 400 MHz




$^1$H NMR: AM1248 Lot N1P21; $CDCl_3$; 400 MHz
CHCl3
0.15
0.10
0.05
1
1
3
8.5
8.0
7.5 Chemical Shift (ppm)


$^1$H NMR: AM1248 Lot N1P21; $CDCl_3$; 400 MHz
0.15
0.10
0.05
1
1
4.6
4.5
4.4
4.3
4.2
4.1
Chemical Shift (ppm)

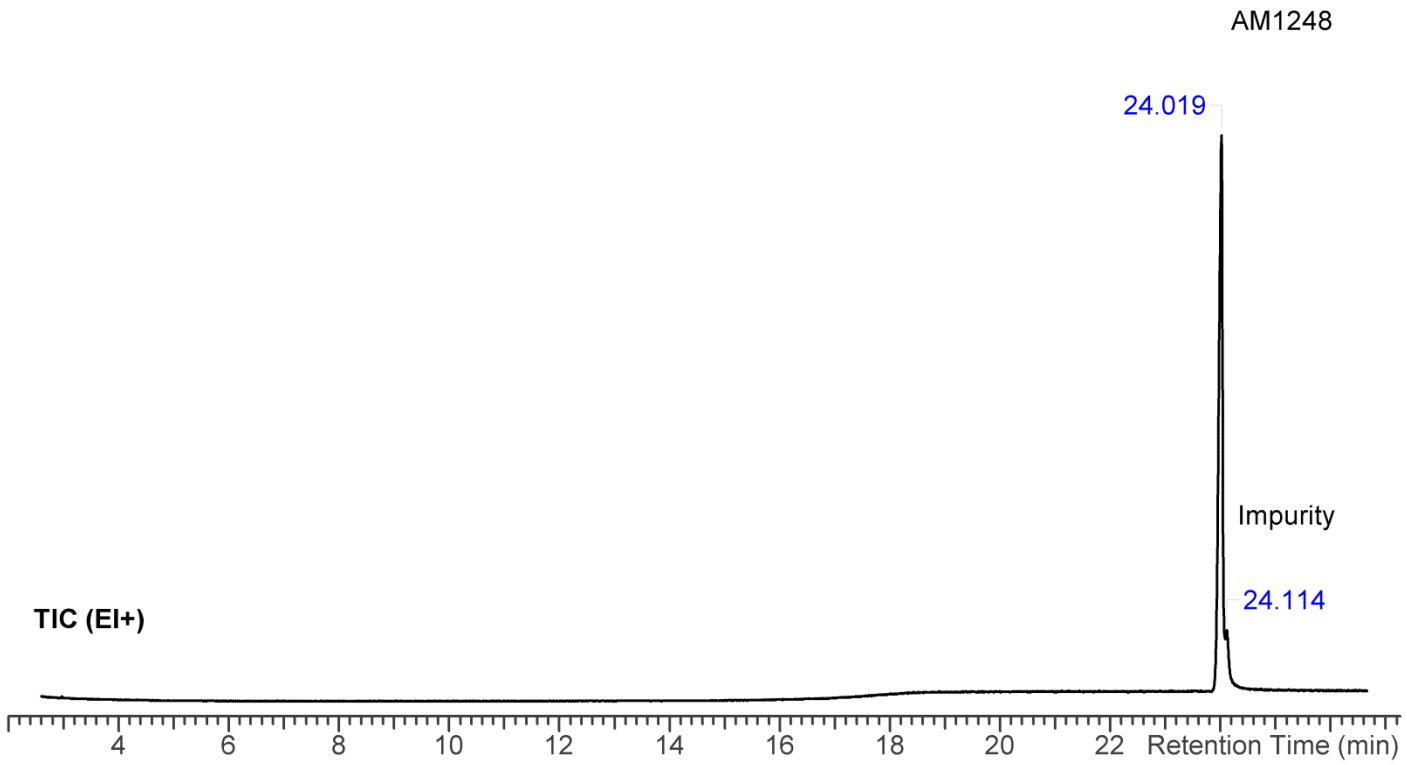

$^1$H NMR: AM1248 Lot N1P21; $CDCl_3$; 400 MHz
0.15
0.10
0.05
1
4
10
6
3
3
3.0
2.5
2.0
1.5
Chemical Shift (ppm)

## 4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

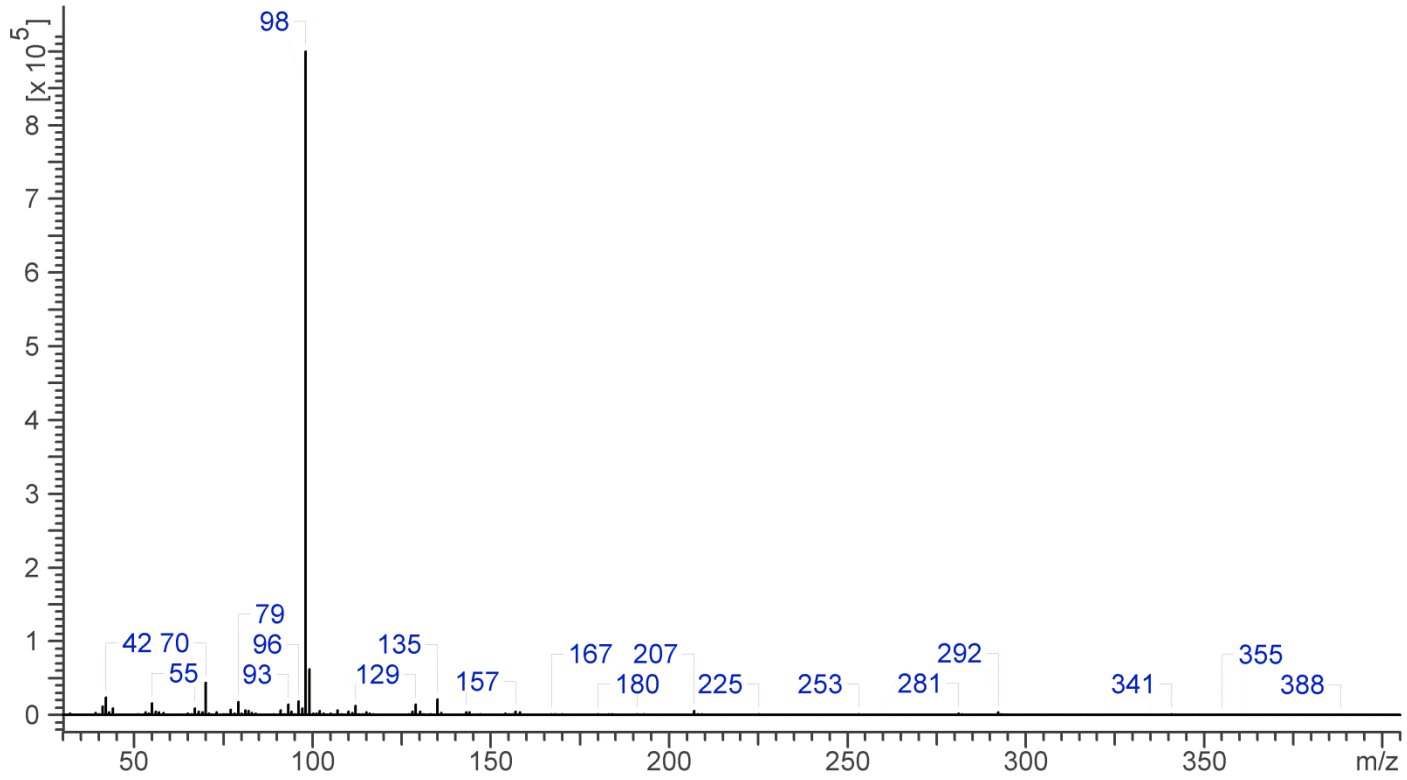
*Sample Preparation:* Dilute analyte to ~1 mg/mL in 9:1 $CHCl_3$:MeOH.

| | |
|---|---|
| ***Instrument:*** | Agilent gas chromatograph operated in split mode with MS detector |
| ***Column:*** | DB-1 MS; 30m x 0.25 mm x 0.25 µm |
| ***Carrier Gas:*** | Helium at 1 mL/min |
| ***Temperatures:*** | Injector: 280°C<br>MSD transfer line: 280°C<br>MS Source: 230°C<br>MS Quad: 150°C<br>Oven program:<br>1) 100°C initial temperature for 1.0 min<br>2) Ramp to 300°C at 12°C/min<br>3) Hold final temperature for 9.0 min |
| ***Injection Parameters:*** | Split Ratio = 20:1, 1 µL injected |
| ***MS Parameters:*** | Mass scan range: 30-550 amu<br>Threshold: 100<br>Tune file: stune.u<br>Acquisition mode: scan |
| ***Retention Time:*** | AM1248 peak at 24.019 min; Impurity peak at 24.114 min |

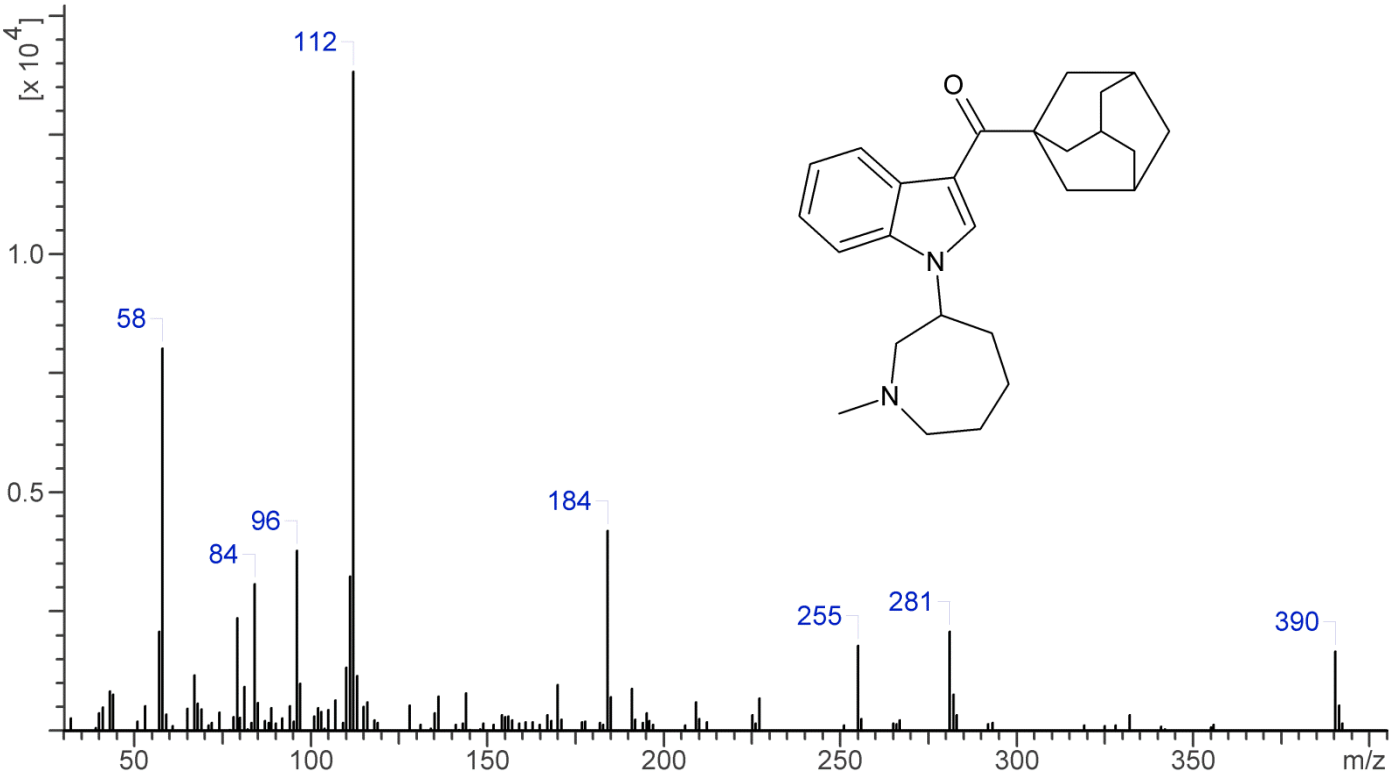
GC/MS TIC: AM1248, Lot N1P21



GC-MS: AM1248; Lot N1P21, 24.019 min




EI Mass Spectrum: AM1248 impurity; lot N1P21, 24.114 min (24.073 min spectrum subtracted)




***GC/MS Observation:***

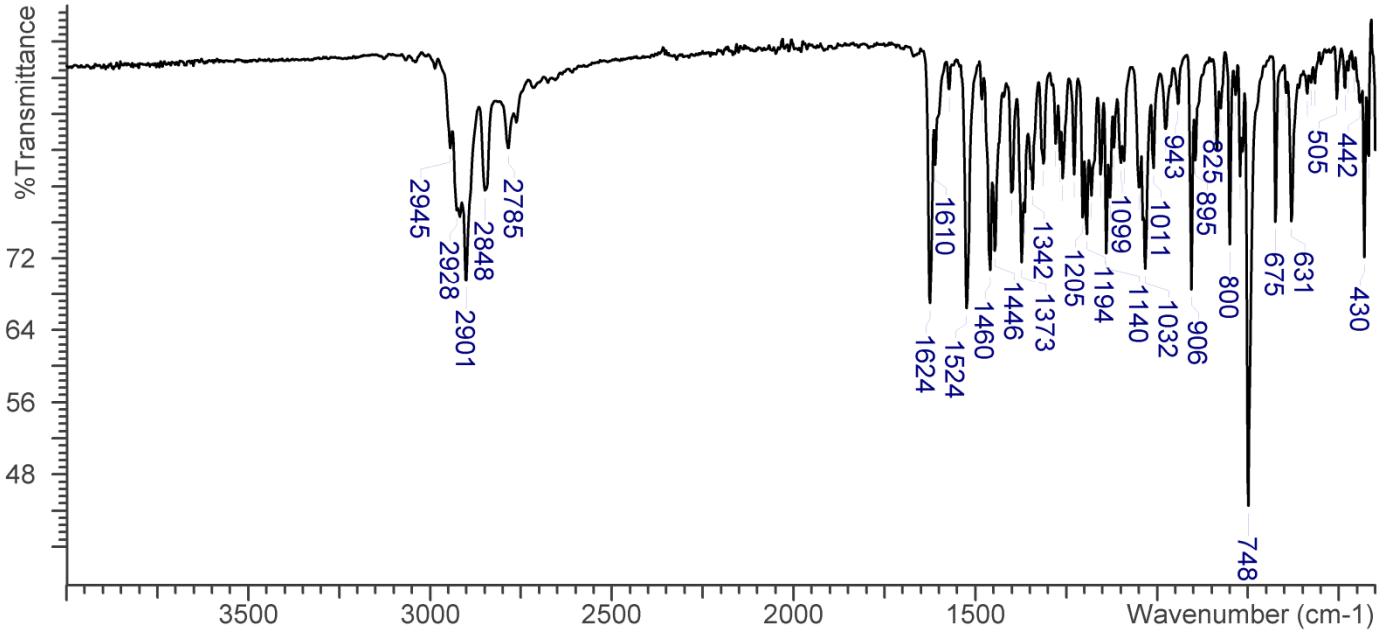
The GC/MS TIC of AM1248 has a shoulder on the right with a dissimilar mass spectrum but the same molecular weight. The major peak at retention time 24.019 minutes is AM1248; while the shoulder at retention time 24.114 minutes is a suspected synthesis byproduct consisting of an azepane isomer. (Citation: "Identification

of the cannabimimetic AM-1220 and its azepane isomer (*N*-methylazepan-3yl)-3-(1-naphthoyl)indole in a research chemical and several herbal mixtures." Forensic Toxicol (2012) 30:126-134)

## 4.3 INFRARED SPECTROSCOPY (FTIR)

***Instrument:*** FTIR with diamond ATR attachment (3 bounce)
***Scan Parameters:*** Number of scans: 32
Number of background scans: 32
Resolution: 4cm$^{-1}$
Sample gain: 8
Aperture: 150

FTIR ATR (Diamond, 3 bounce): AM1248; Lot N1P21




FTIR ATR (Diamond, 3 bounce): AM1248; Lot N1P21