

1. GENERAL INFORMATION

IUPAC Name: (2-iodophenyl)(1-pentyl-1*H*-indol-3-yl)-methanone

CAS#: 335160-91-3

Synonyms: 1-pentyl-3-(2-iodobenzoyl)indole

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 ₂₀ H ₂₀ INO	417	89.6

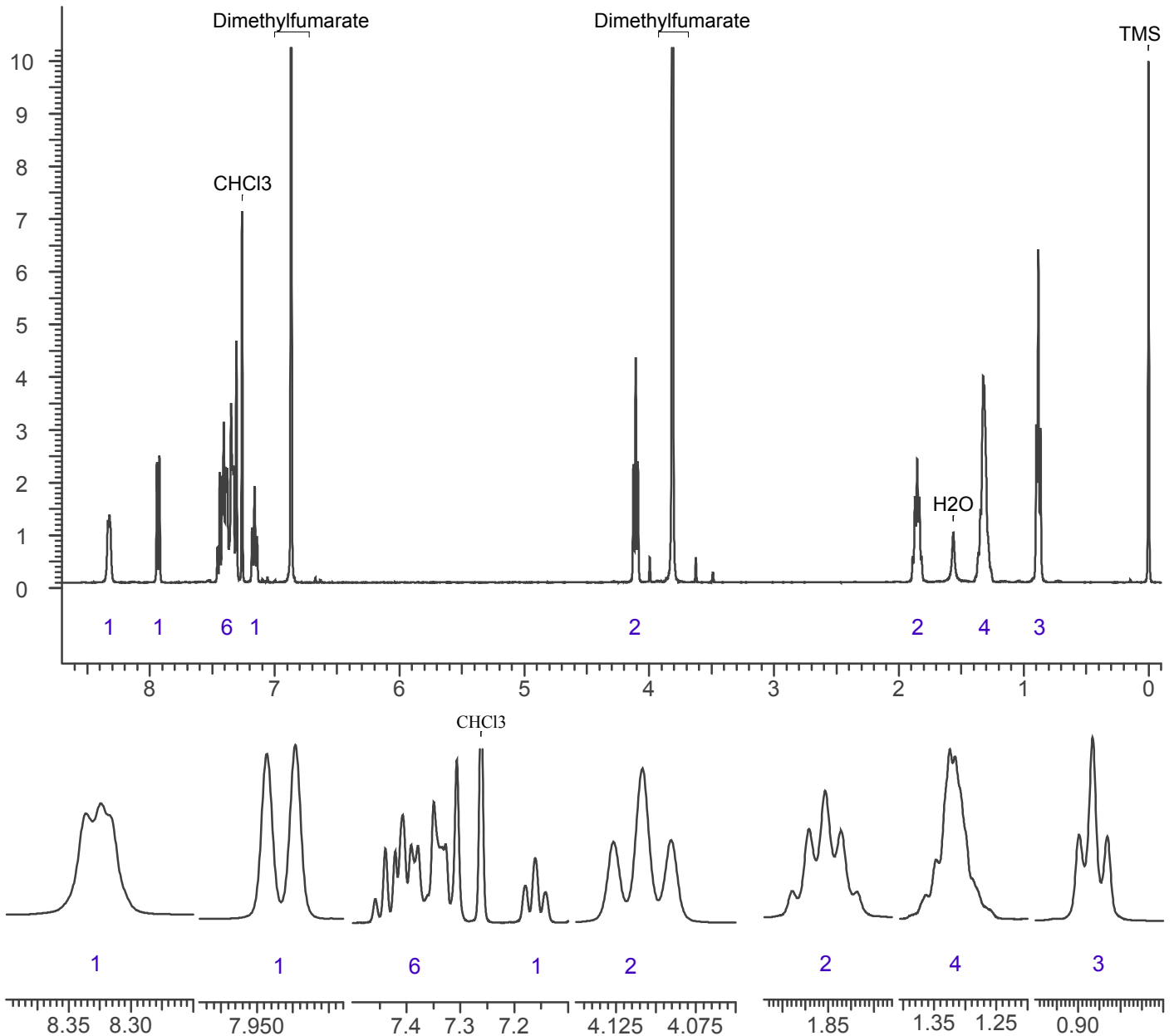
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~5 mg/mL in CDCl₃ containing TMS for 0 ppm reference and dimethylfumarate 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

¹H NMR, AM-679 Lot # 0437656-5, CDCl₃, 400MHz





AM-679

This peer reviewed document may be used for the verification or identification of drug materials (subject to laboratory policy).



3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

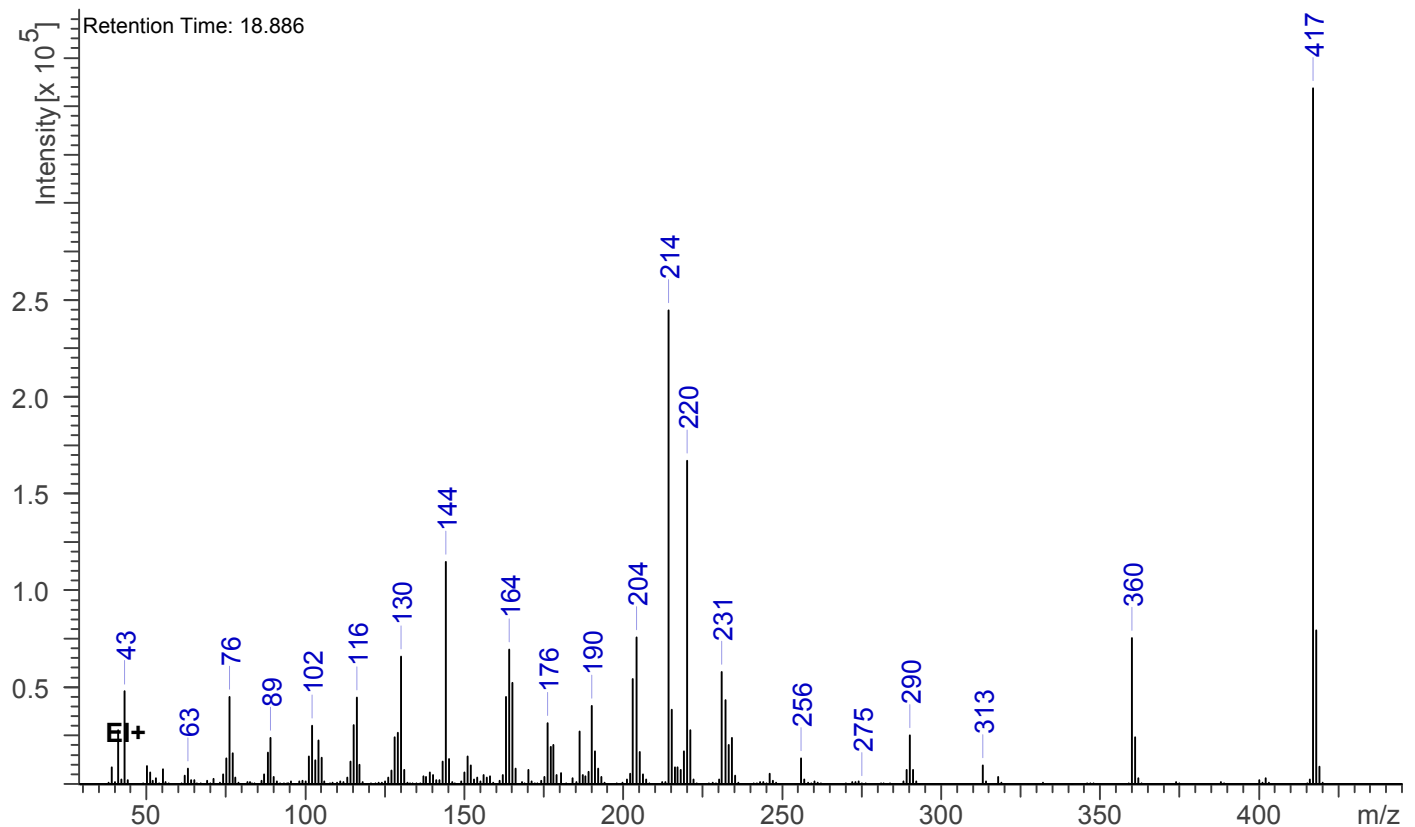
Sample Preparation: Dilute analyte ~5 mg/mL in chloroform.

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 μ m
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 30.0 min

Injection Parameters: Split Ratio = 20:1, 1 μ L injected
MS Parameters: Mass scan range: 30-550 amu
Threshold: 100
Tune file: stune.u
Acquisition mode: scan

Retention Time: 18.868 min

EI Mass Spectrum, AM-679 Lot # 0437656-5





AM-679

This peer reviewed document may be used for the verification or identification of drug materials (subject to laboratory policy).

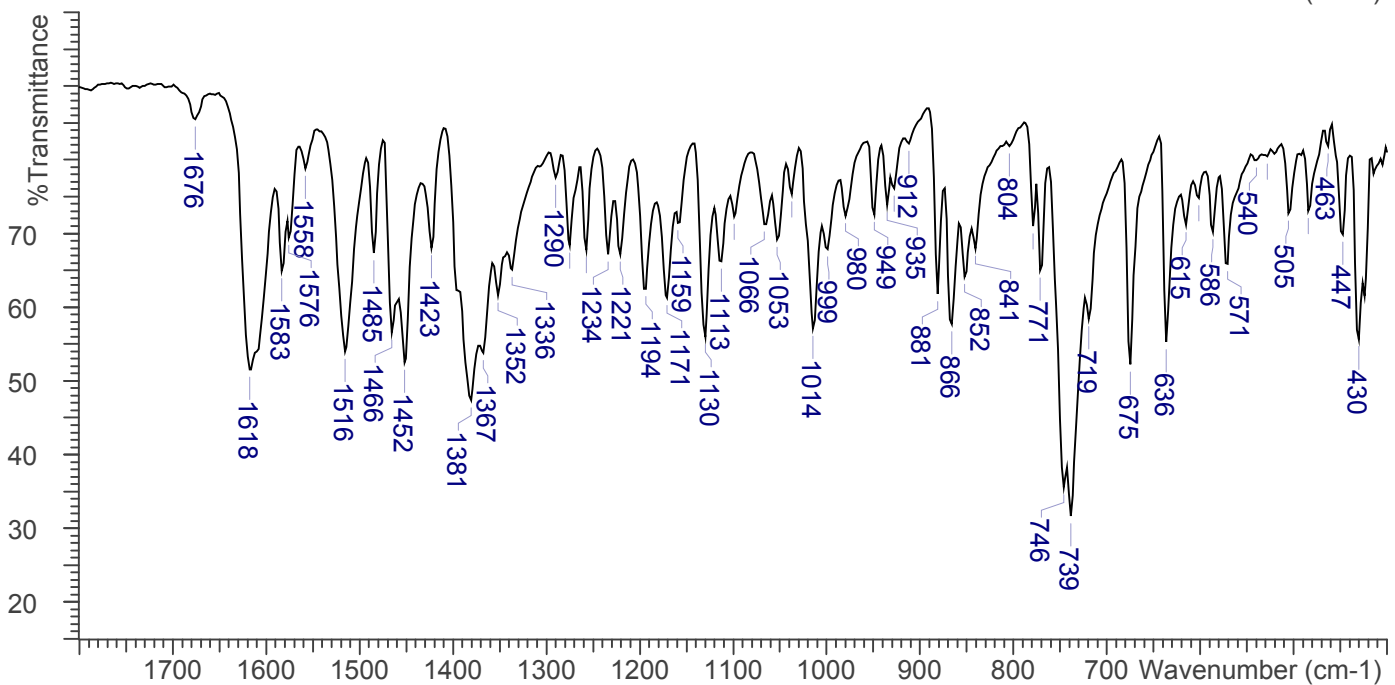
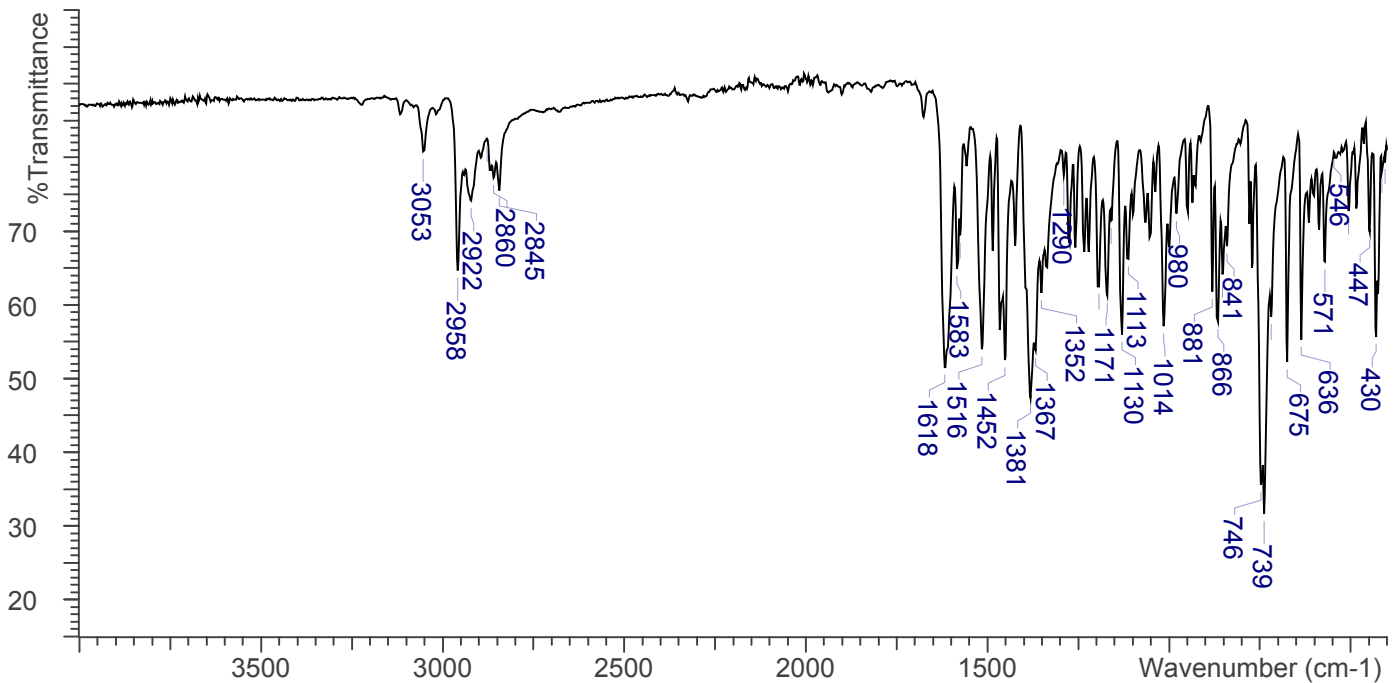


3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: 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) AM-679 Lot # 0437656-5





AM-679

This peer reviewed document may be used for the verification or identification of drug materials (subject to laboratory policy).



4. ADDITIONAL RESOURCES

[Forendex](#)

[Wikipedia](#)