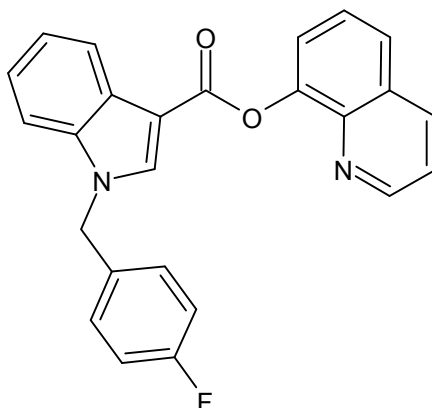




FUB-PB-22

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



1. GENERAL INFORMATION

IUPAC Name: quinolin-8-yl 1-(4-fluorobenzyl)-1H-indole-3-carboxylate

CAS#: Not Available

Synonyms: Not Available

Source: DEA Reference Material Collection

Appearance: White Powder

UV_{max} (nm): Not Available

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₂₅ H ₁₇ FN ₂ O ₂	396	172.4



FUB-PB-22

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



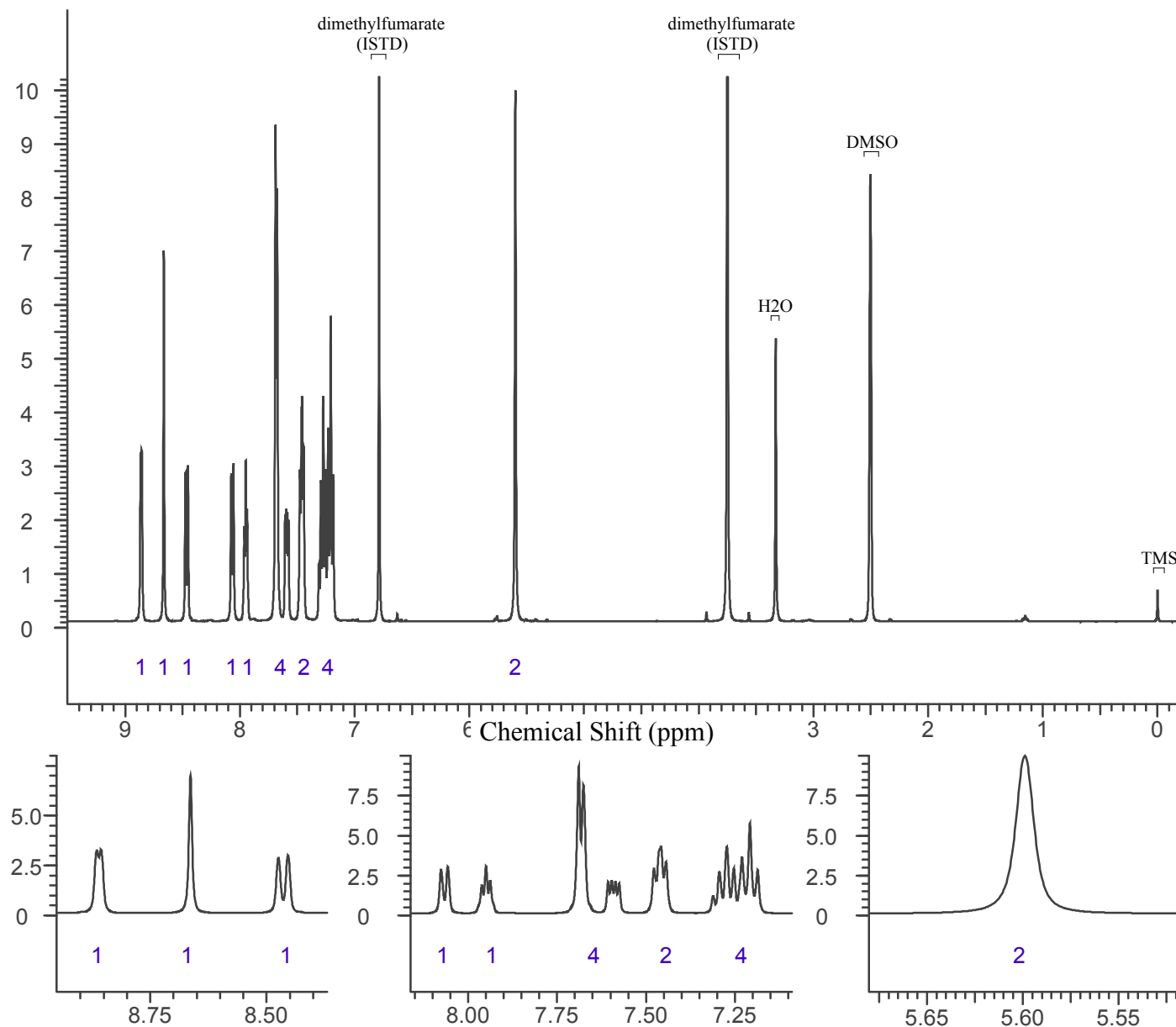
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~15 mg/mL in dimethylsulfoxide (DMSO) 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: FUB-PB-22 Lot# RM-131008-01; DMSO; 400MHz





FUB-PB-22

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



3.2 Gas Chromatography/Mass Spectrometry

Sample Preparation: Dilute analyte ~ 4 mg/mL into 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 25.0 min

Injection Parameters: Split Ratio = 20:1, 1 μ L injected

MS Parameters: Mass scan range: 34-550 amu

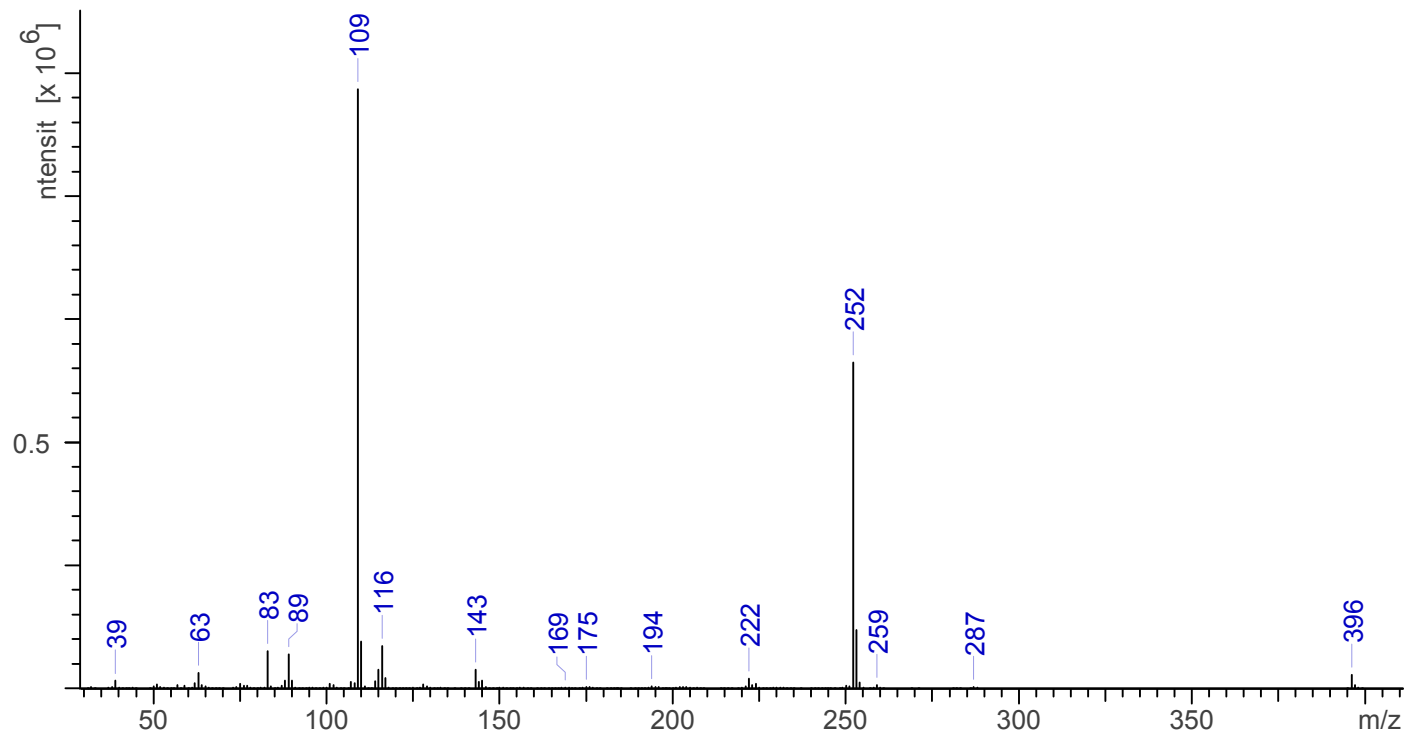
Threshold: 90

Tune file: stune.u

Acquisition mode: scan

Retention Time: 23.105 min

EI Mass Spectrum: FUB-PB-22 Lot# RM-131008-01





FUB-PB-22

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

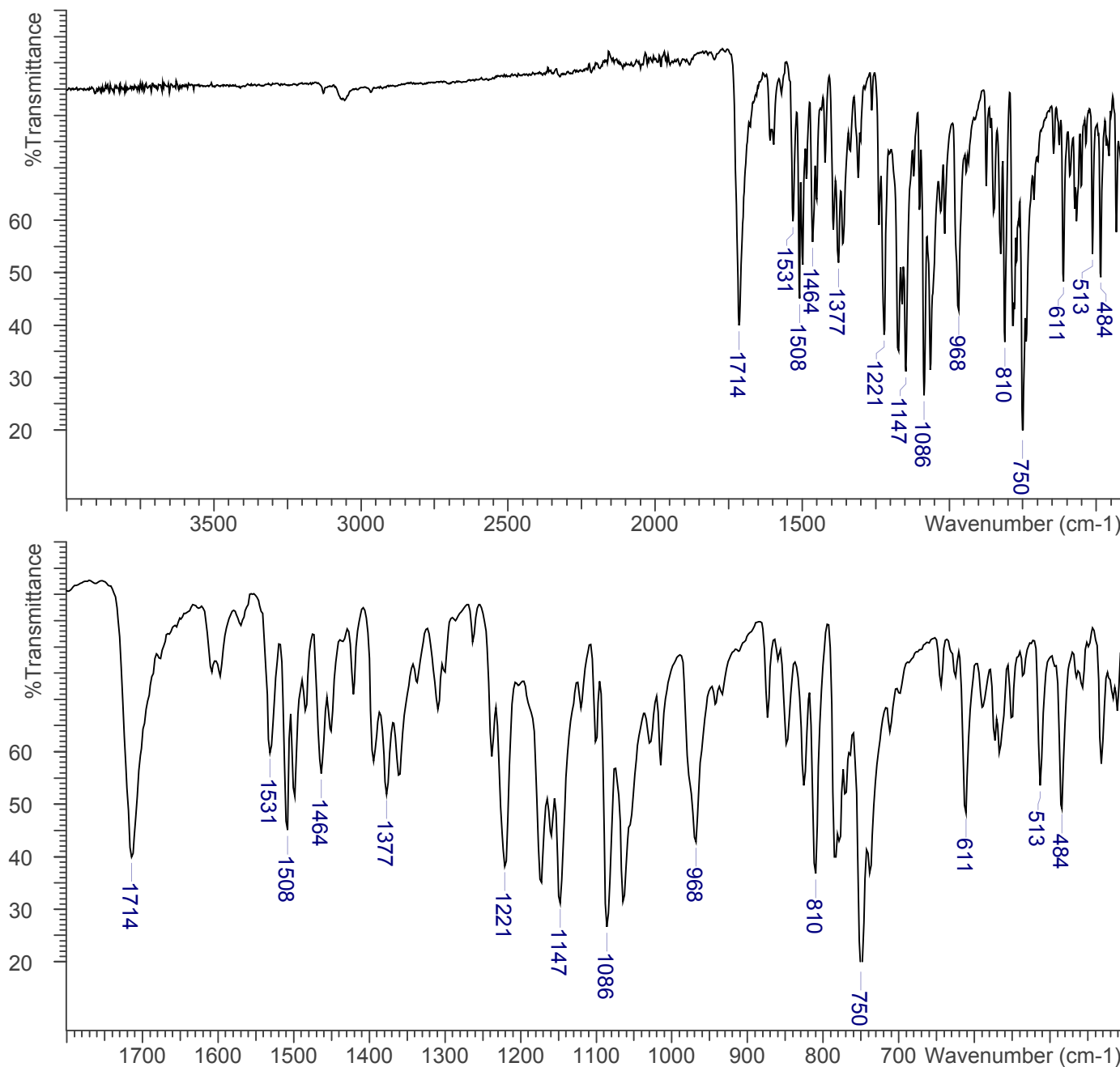


3.3 INFRARED SPECTROSCOPY (FTIR)

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): FUB-PB-22 Lot# RM-131008-01





FUB-PB-22

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



4. ADDITIONAL RESOURCES

No resources identified as of 02/19/14