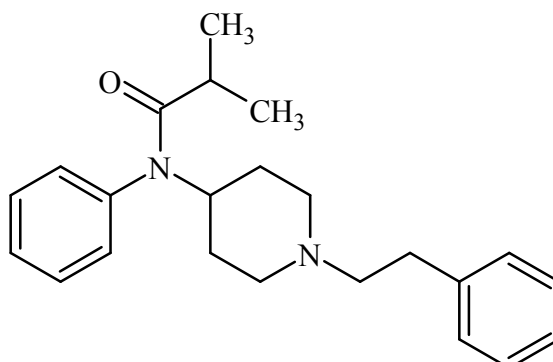




Isobutyryl fentanyl

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



1. GENERAL INFORMATION

IUPAC Name:	2-methyl-N-phenyl-N-[1-(2-phenylethyl)piperidin-4-yl]propanamide
CAS#:	117332-90-8 (HCl)
Synonyms:	N-(1-Phenethylpiperidin-4-yl)N-phenylisobutyramide, NIH 10487
Source:	DEA Reference Material Collection
Appearance:	white powder
UV_{max}(nm):	NA

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₂₃ H ₃₀ N ₂ O	350.50	NA
HCl	C ₂₃ H ₃₀ N ₂ O · HCl	386.96	NA



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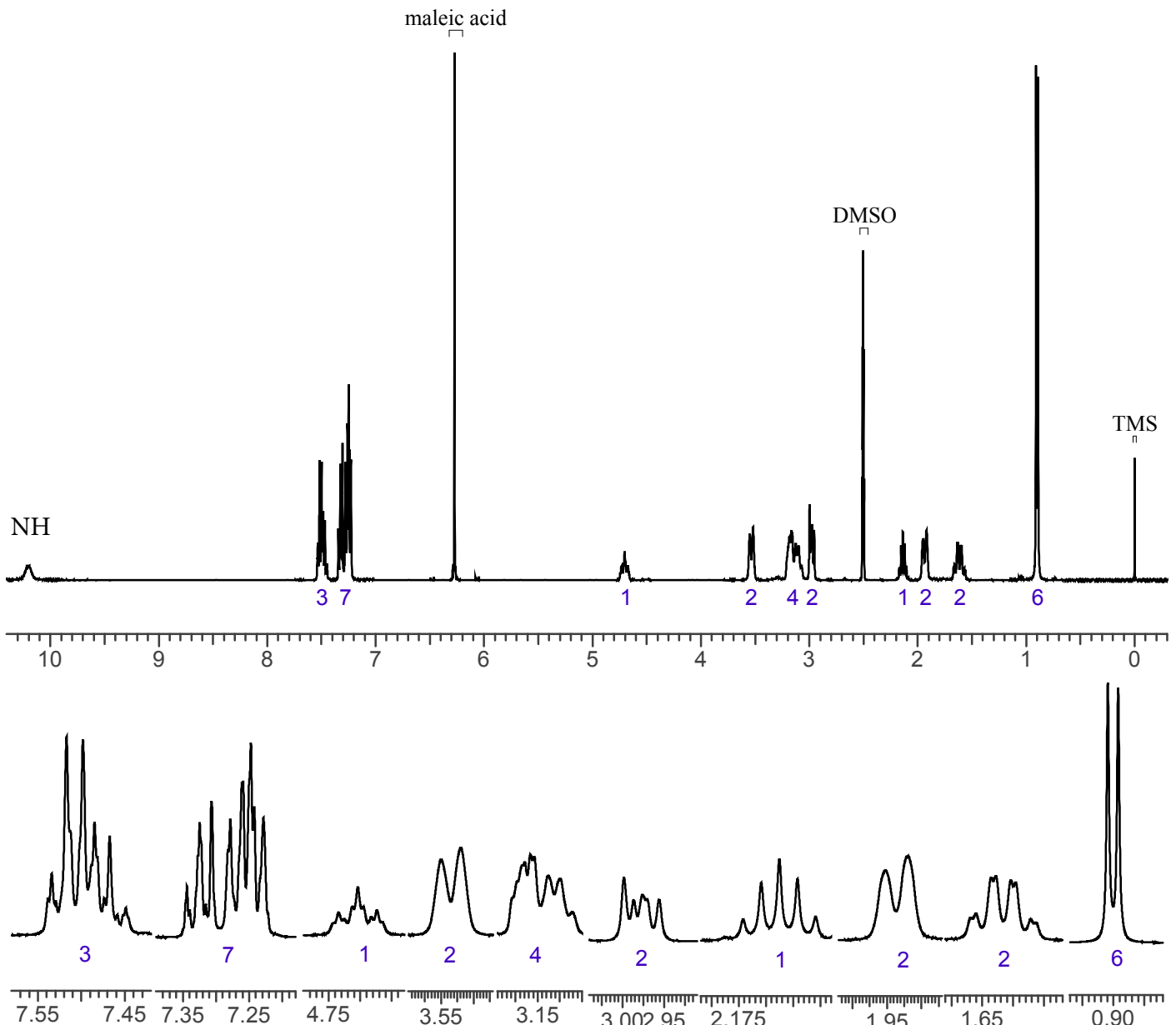
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~11 mg/mL in DMSO-d₆ containing TMS for 0 ppm reference and maleic acid 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

¹HNMR: Isobutyryl fentanyl HCl Lot# ALB-235-7; DMSO-d₆; 400 MHz





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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL into methanol.

Instrument: Agilent gas chromatograph operated in split mode with MS detector

Column: HP-5; 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 280°C at 12 °C/min

3) Hold final temperature for 9.0 min

Injection Parameters: Split Ratio = 25:1, 1 μ L injected

MS Parameters: Mass scan range: 30-550 amu

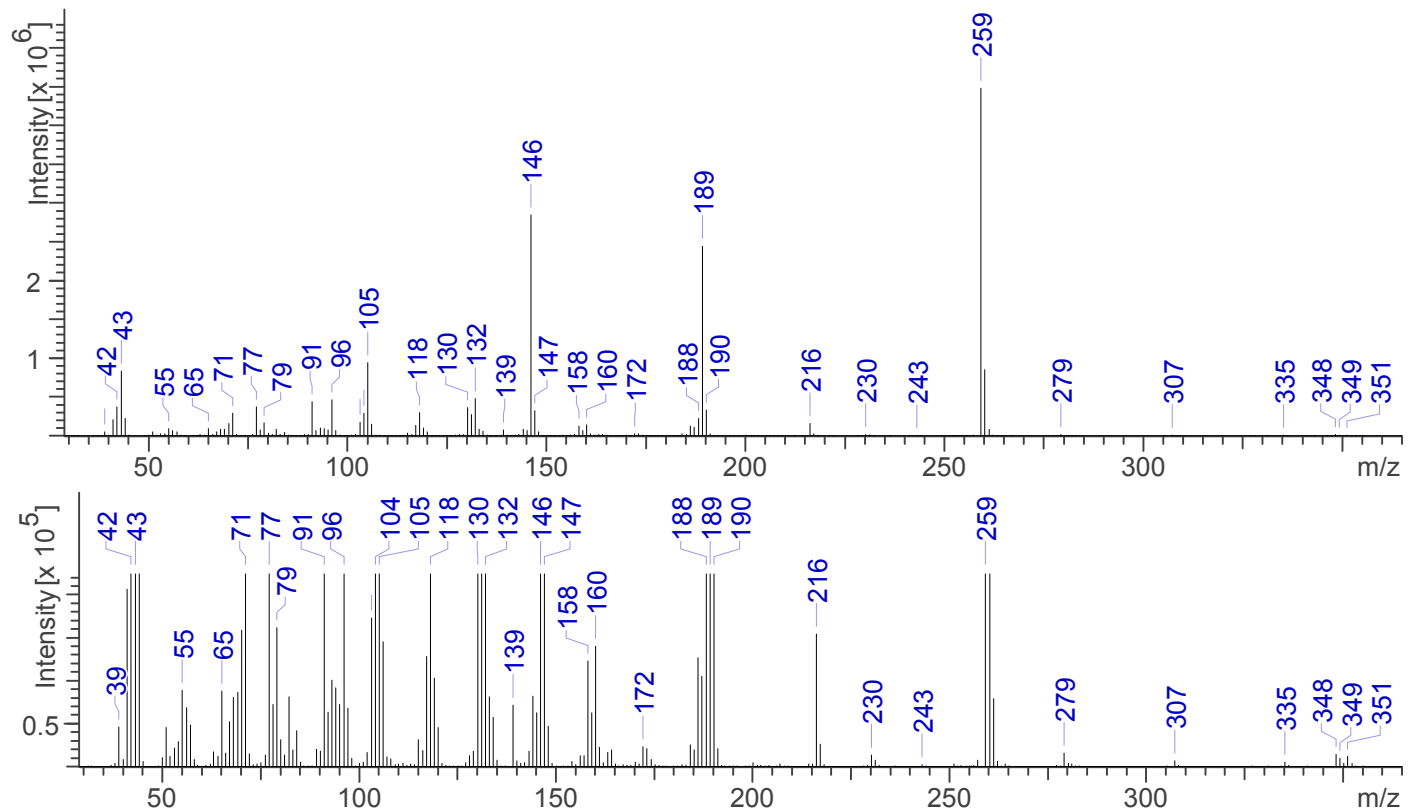
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

Retention Time: 16.946 min

EI Mass Spectrum: Isobutyryl fentanyl HCl Lot# ALB-235-7





Isobutyryl fentanyl



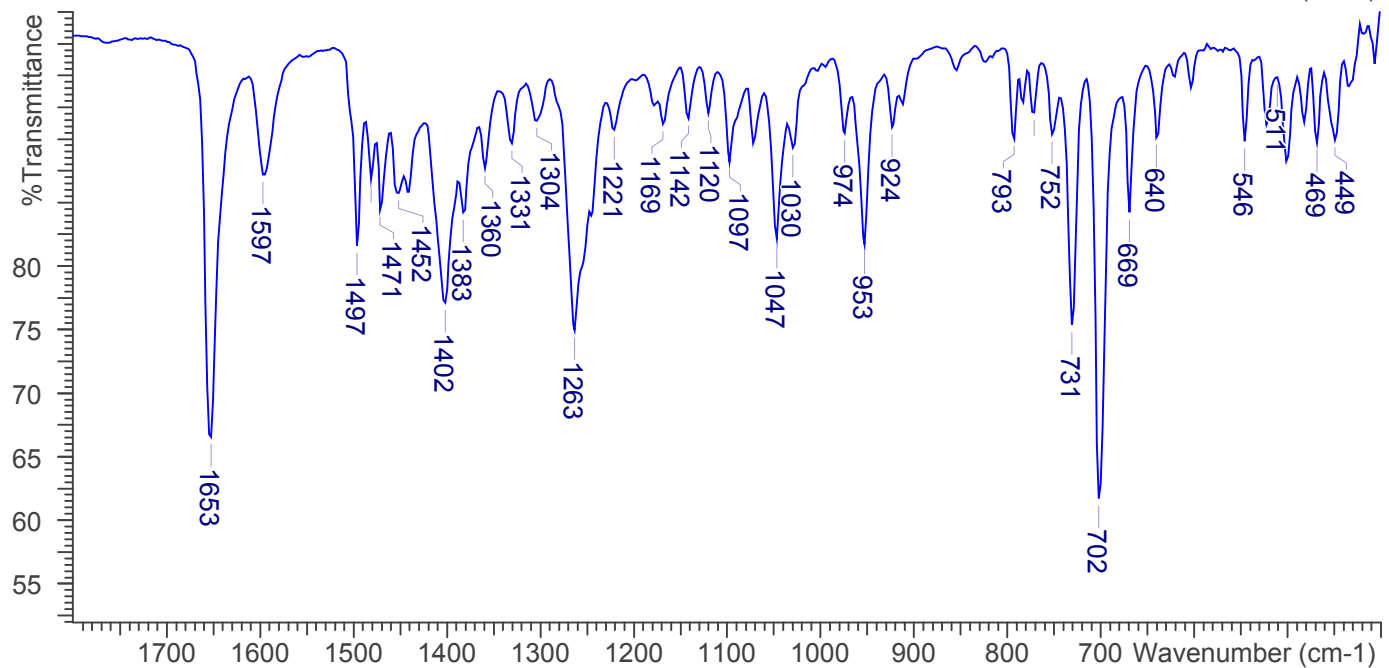
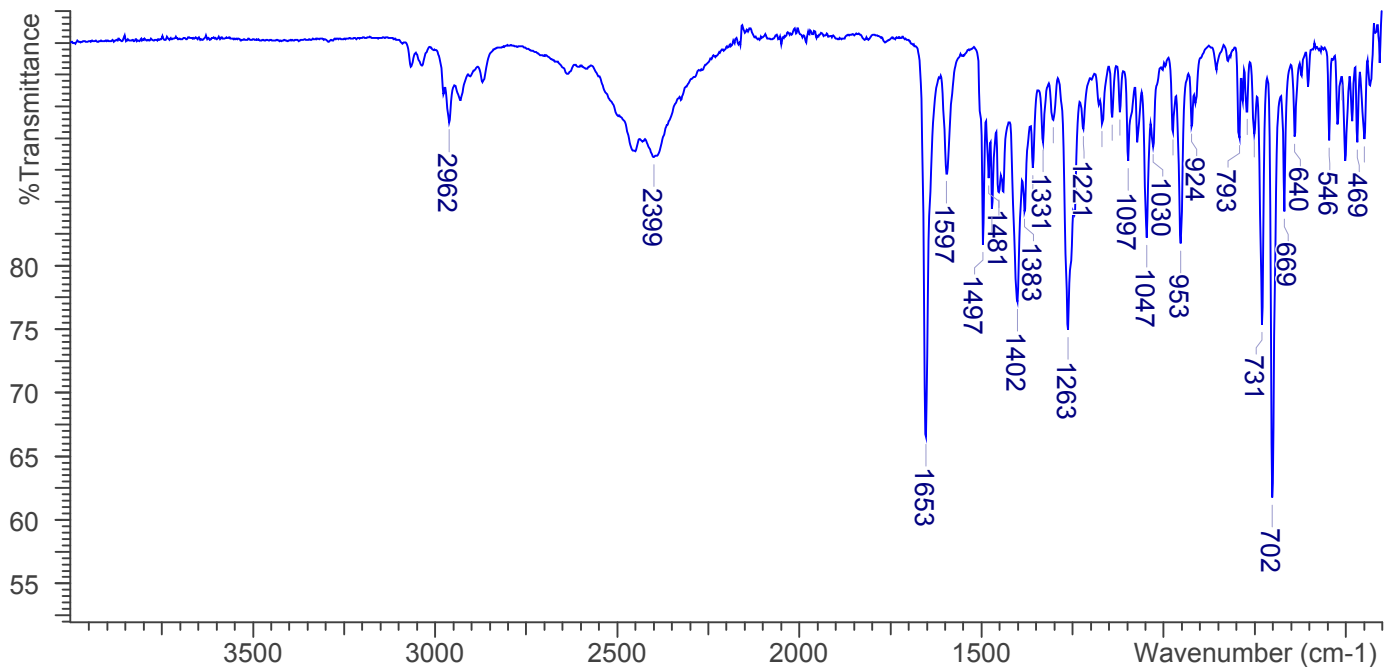
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3.3 INFRARED SPECTROSCOPY (FTIR)

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: Isobutyryl fentanyl HCl Lot# ALB-235-7





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4. ADDITIONAL RESOURCES

No additional resources as of 05/30/17