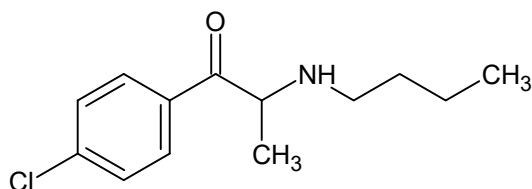




4-Chlorobutylcathinone

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



1. GENERAL INFORMATION

IUPAC Name:	2-(butylamino)-1-(4-chlorophenyl)propan-1-one
CAS#:	N/A
Synonyms:	N-butyl-4-chlorocathinone, 1-(4-chlorophenyl)-2-(butylamino)propan-1-one
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 ₁₃ H ₁₈ ClNO	239.74	Not Determined
HCl	C ₁₃ H ₁₈ ClNO HCl	276.20	212.8-213.4



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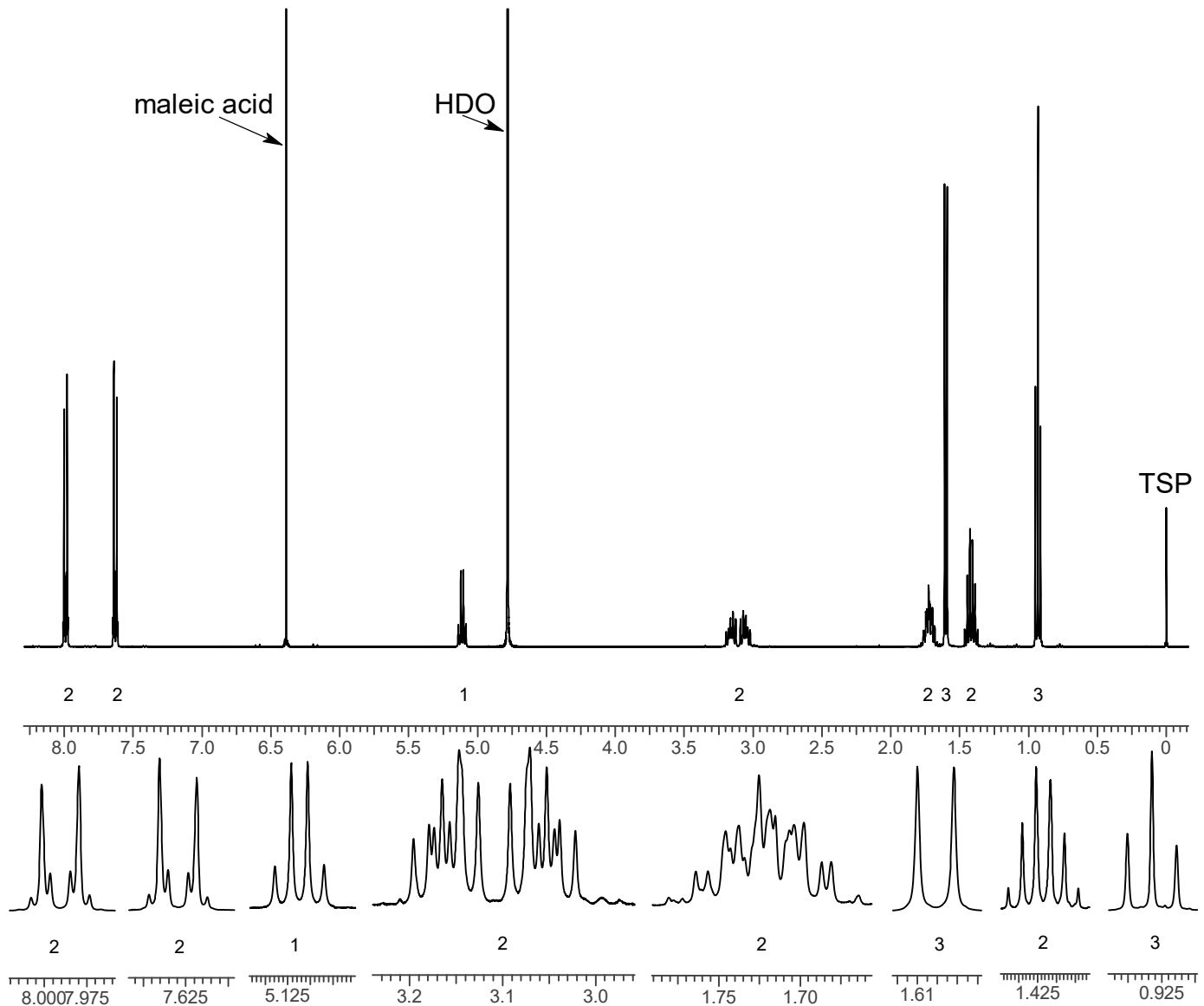
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~15 mg/2mL in D₂O containing TSP 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: 4-Chlorobutylcathinone HCl; Lot# RM-160811-01; D₂O; 400MHz





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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~3 mg/mL in CHCl₃, base extracted

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

Column: HP-5 MS (or equivalent); 30m x 0.25 mm x 0.25 μm

Carrier Gas: Helium at 1.5 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

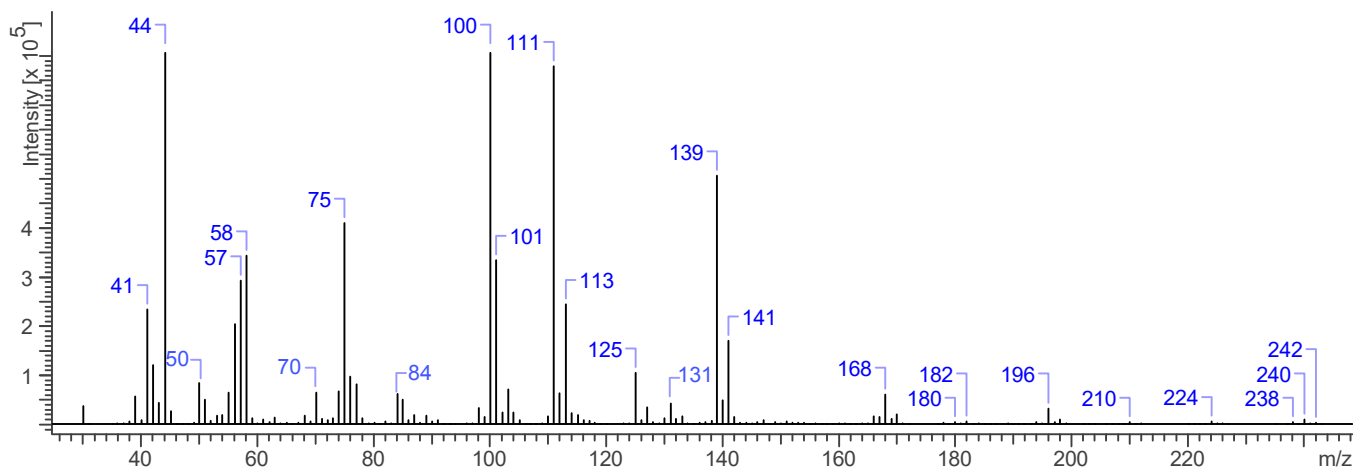
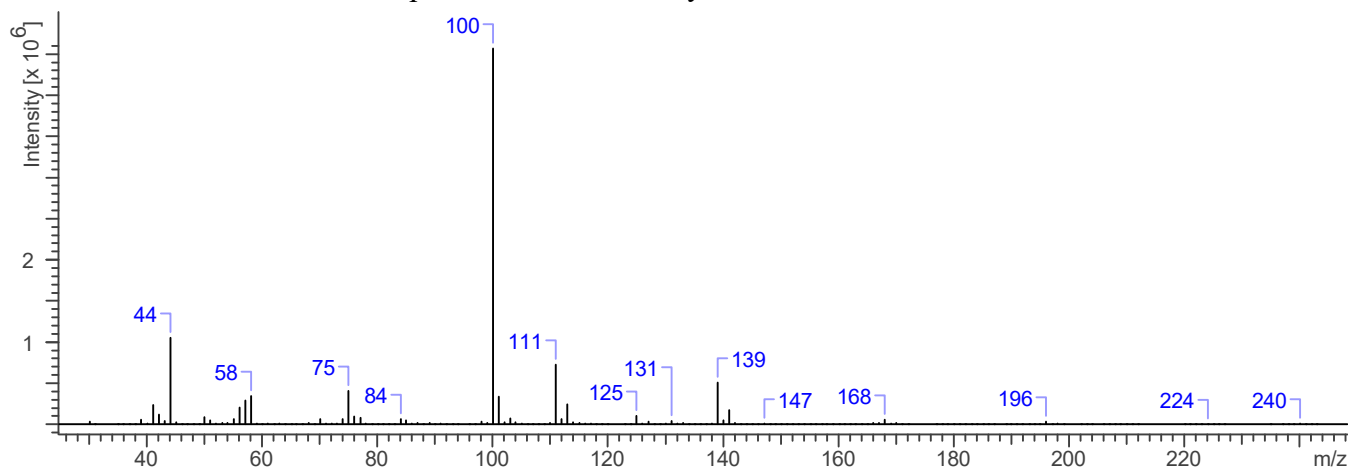
Injection Parameters: Split Ratio = 25:1, 1 μL injected

MS Parameters: Mass scan range: 30-550 amu Threshold: 250

Tune file: stune.u Acquisition mode: scan

Retention Time: 9.53 min

EI Mass Spectrum: 4-Chlorobutylcathinone HCl; Lot# RM-160811-01





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3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (1 bounce)

Scan Parameters:
Number of scans: 32
Number of background scans: 32
Resolution: 4 cm⁻¹
Sample gain: 1
Aperture: 150

FTIR ATR (Diamond 1 Bounce): 4-Chlorobutylcathinone HCl; Lot# RM-160811-01

