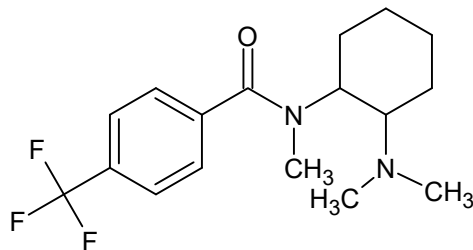




4-(Trifluoromethyl) U-47700

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



1. GENERAL INFORMATION

IUPAC Name:	<i>N</i> -[2-(dimethylamino)cyclohexyl]- <i>N</i> -methyl-4-(trifluoromethyl)benzamide
CAS#:	2836411-48-2 (HCl)
Synonyms:	4-TFM U-47700, <i>N</i> -((1 <i>R</i> ,2 <i>R</i>)-2-(dimethylamino)cyclohexyl)- <i>N</i> -methyl-4-(trifluoromethyl)benzamide
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)
Hydrochloride	C ₁₇ H ₂₃ F ₃ N ₂ O HCl	364.83	N/A
Base	C ₁₇ H ₂₃ F ₃ N ₂ O	328.37	N/A



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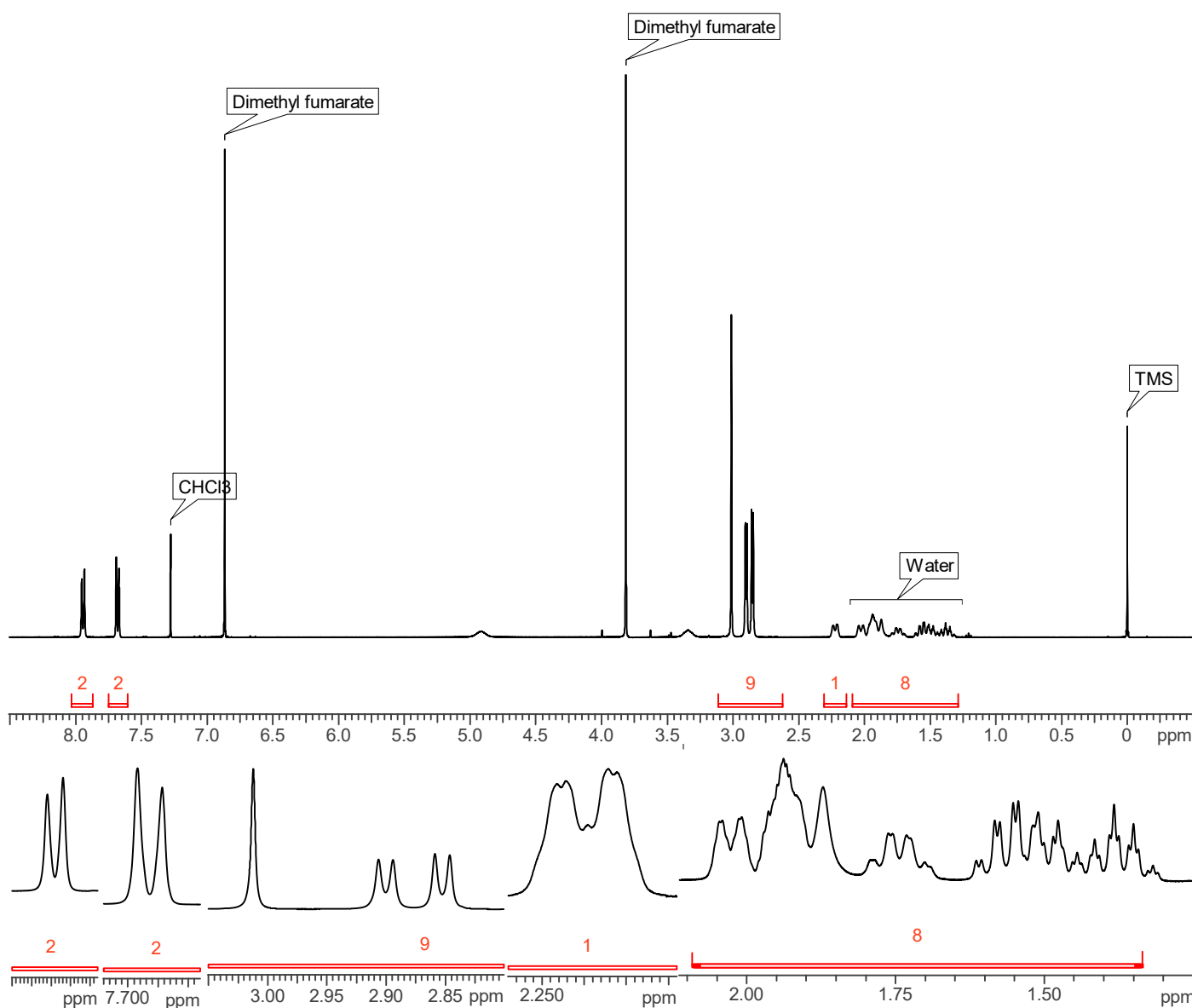
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~11 mg/mL in CDCl_3 containing TSP for 0 ppm reference and dimethyl fumarate 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: 4-(Trifluoromethyl) U-47700 HCl; Lot# 0603861-7; CDCl_3 ; 400 MHz





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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

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 μ m
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 μ L injected

MS Parameters: Mass scan range: 30-550 amu

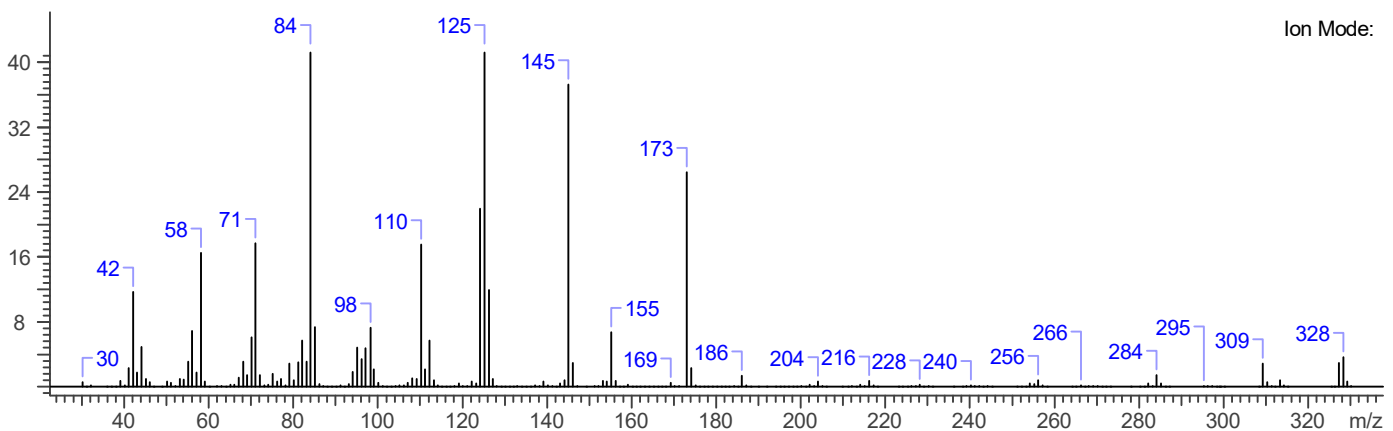
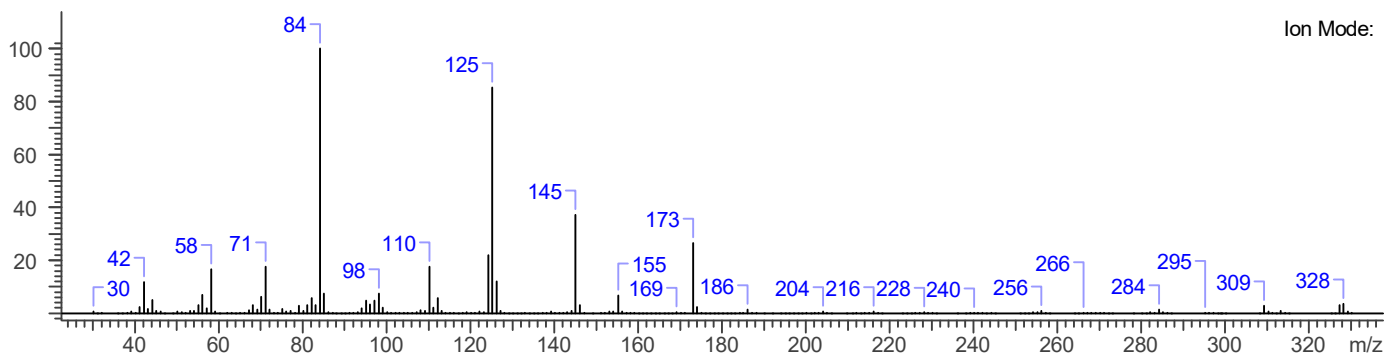
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

Retention Time: 11.359 min

EI Mass Spectrum: 4-(Trifluoromethyl) U-47700 HCl; Lot#0603861-7





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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: 4
Aperture: 150

FTIR ATR (Diamond 1 Bounce): 4-(Trifluoromethyl) U-47700 HCl; Lot# 0603861-7

