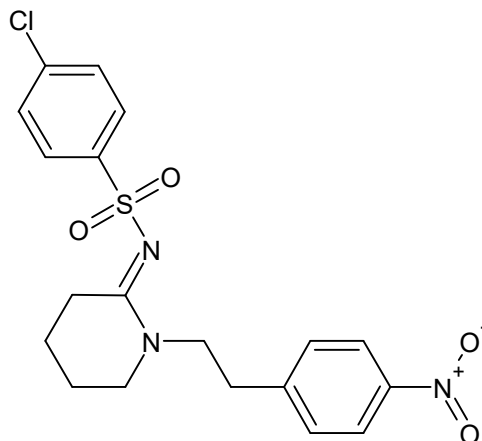




W-18

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



1. GENERAL INFORMATION

IUPAC Name:	4-chloro- <i>N</i> -{(2 <i>E</i>)-1-[2-(4-nitrophenyl)ethyl]piperidin-2-ylidene}-benzenesulfonamide
CAS#:	93101-02-1
Synonyms:	1-(4-nitrophenyl)ethylpiperidylidene-2-(4-chlorophenyl)sulfonamide
Source:	DEA Reference Material Collection
Appearance:	Yellow 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 ₁₉ H ₂₀ ClN ₃ O ₄ S	421	162.6

2.2 Analytical Observations

W-18 exhibits limited solubility in methanol.



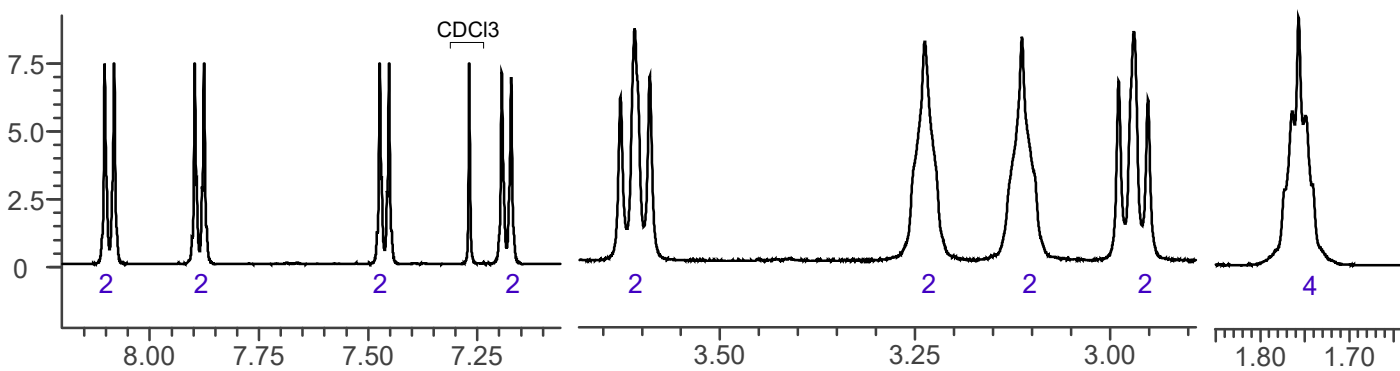
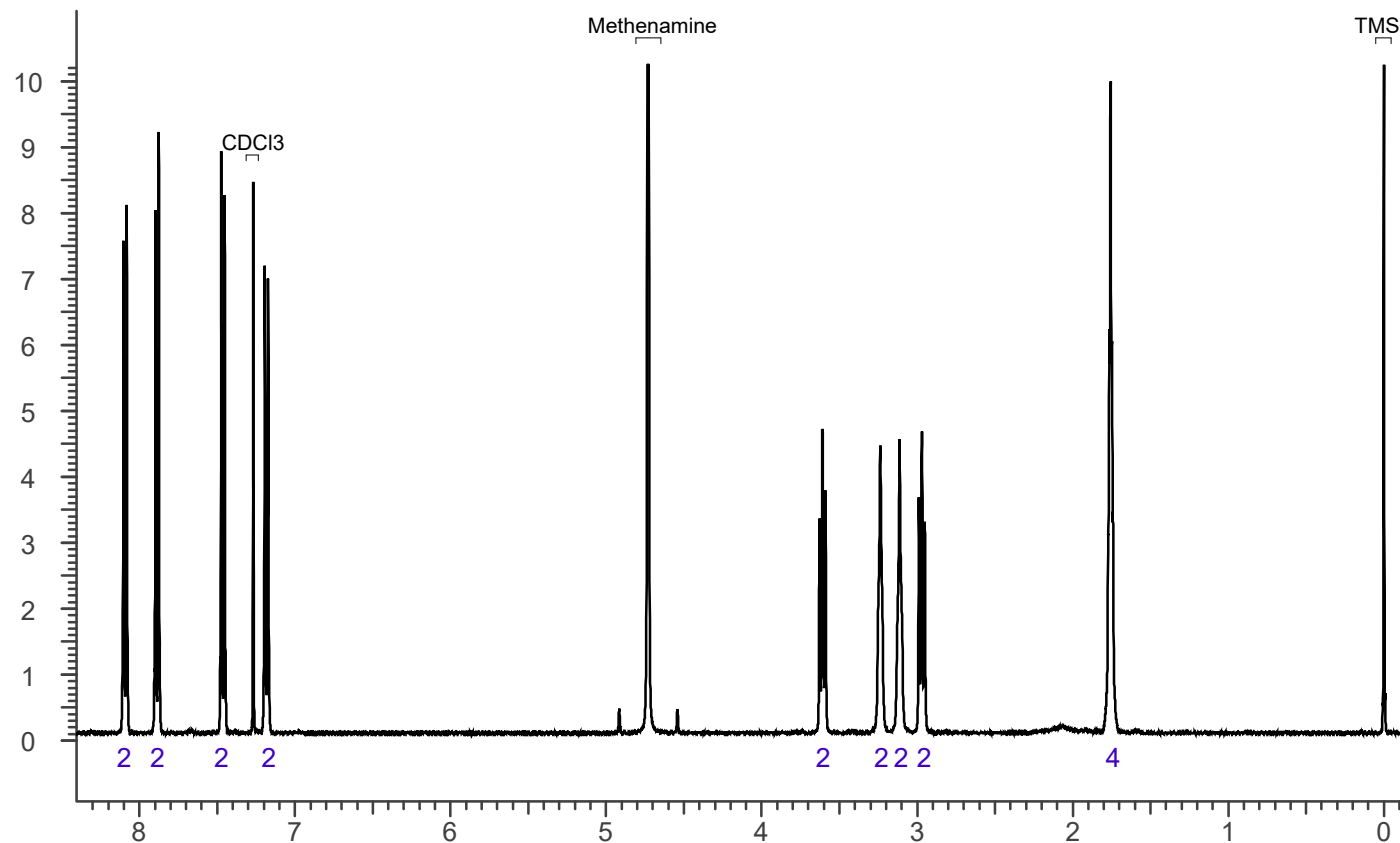
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~11 mg/mL in CDCl₃ containing TMS for 0 ppm reference and methenamine 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: W-18 Lot#RM-131001-01, CDCl₃, 400MHz





W-18

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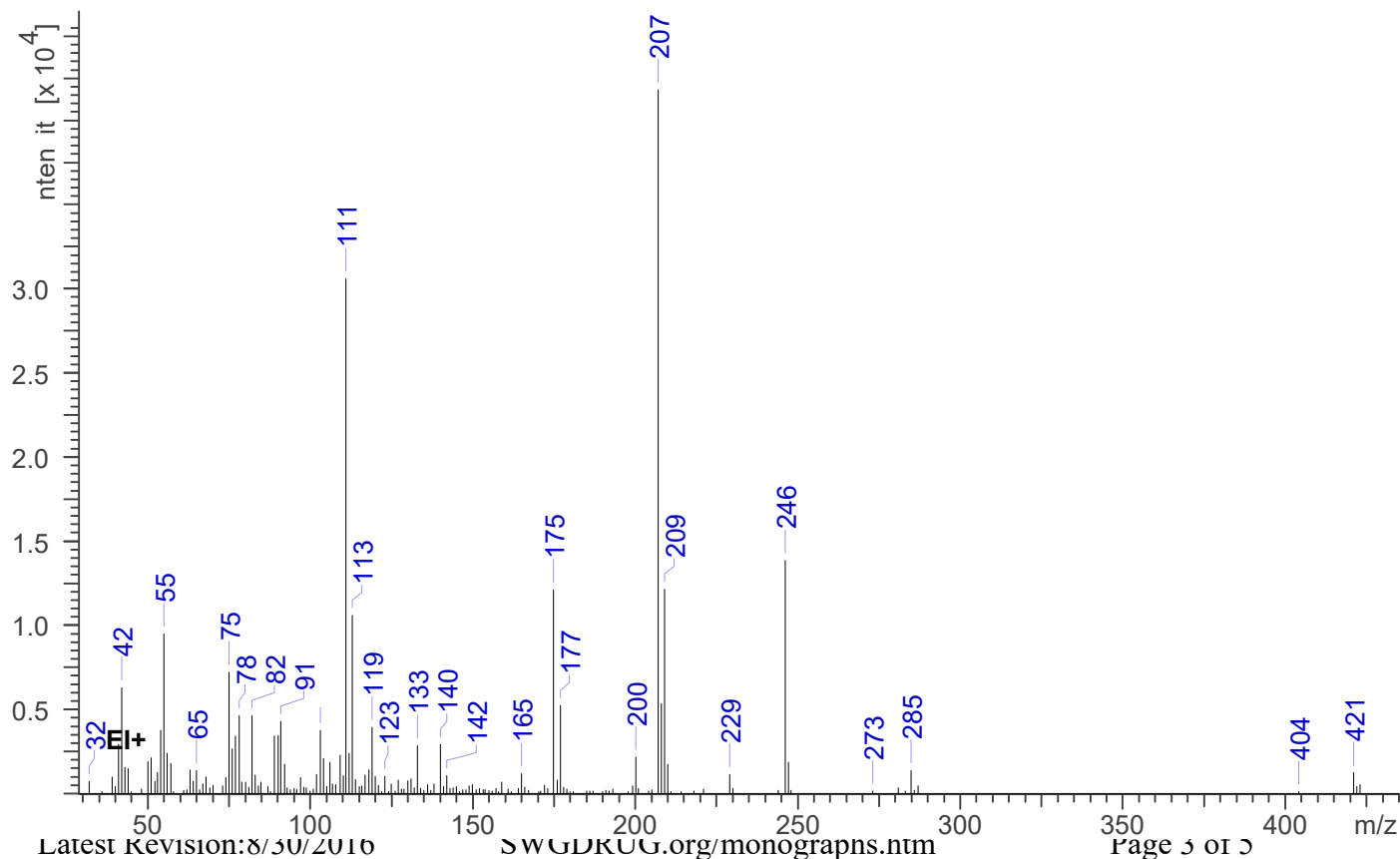
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in CHCl₃.

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 μm
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 = 25:1, 1 μL injected
MS Parameters: Mass scan range: 30-550 amu
Threshold: 100
Tune file: stune.u
Acquisition mode: scan
Retention Time: 25.476 min

EI Mass Spectrum: W-18 Lot#RM-131001-01





W-18

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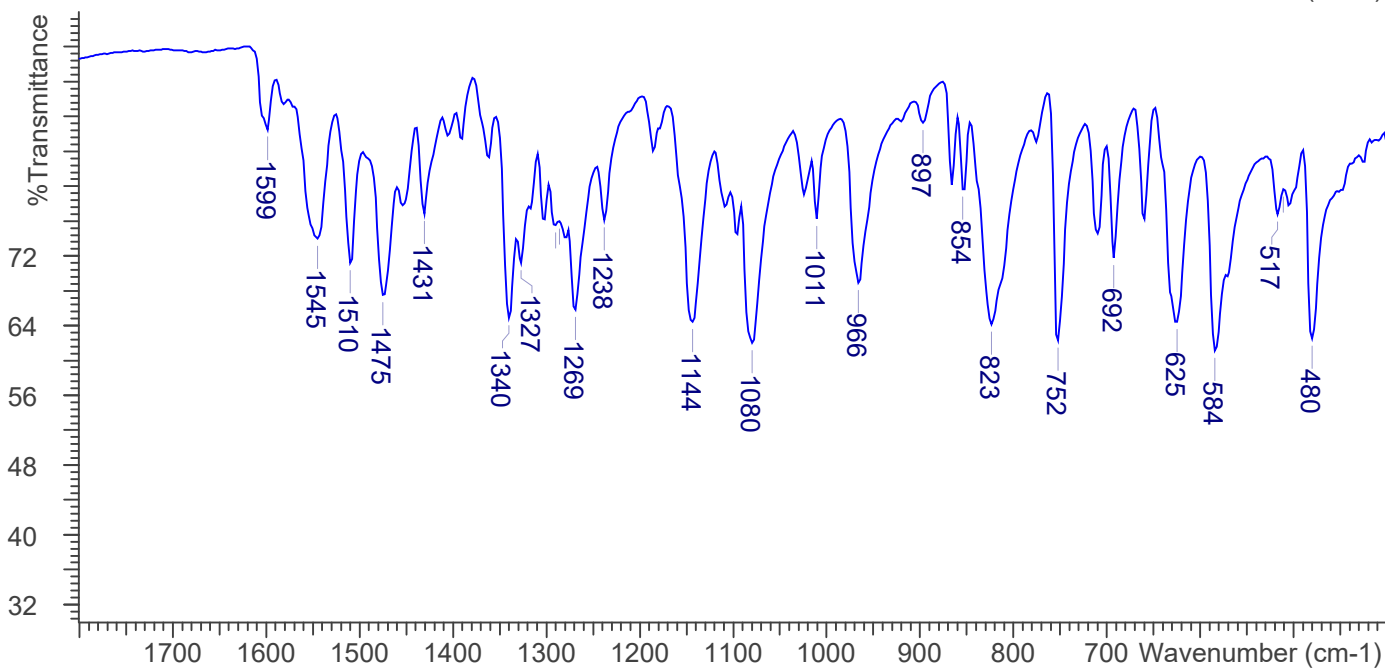
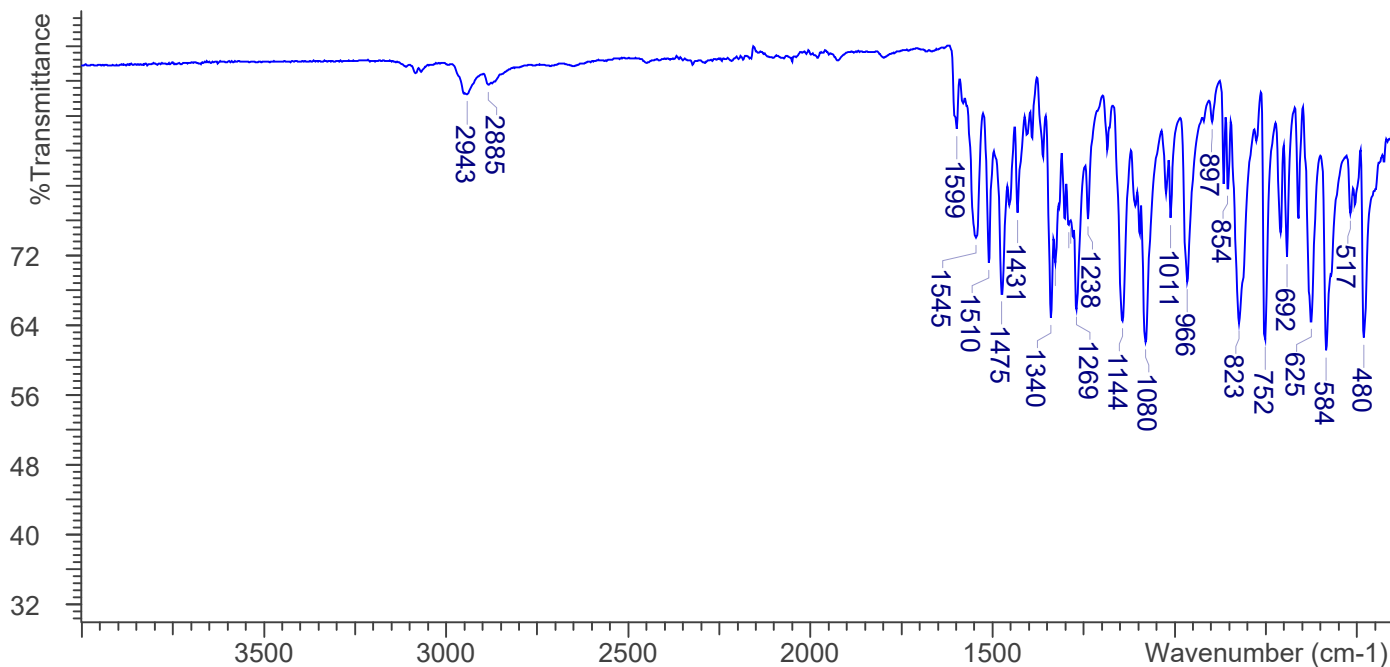


3.3 INFRARED SPECTROSCOPY (FTIR)

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: 8
Aperture: 150

FTIR ATR (Diamond, 1 Bounce): W-18 Lot#RM-131001-01





W-18

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4. ADDITIONAL RESOURCES

[Wikipedia](#)