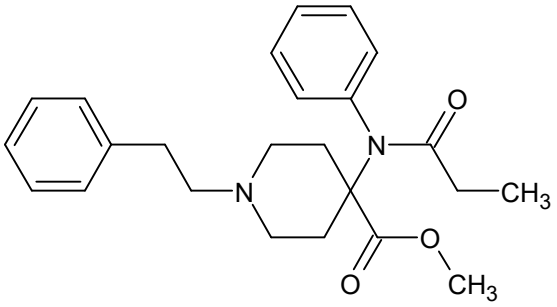
Carfentanil

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



1. GENERAL INFORMATION

IUPAC Name: methyl 1-(2-phenylethyl)-4-[phenyl(propanoyl)amino]piperidine-4-carboxylate

CAS#: 59708-52-0

Synonyms: carfentanyl

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 (^{o}C)
Base	$C_{24}H_{30}N_2O_3$	394.50	Not Determined
Citrate	$C_{24}H_{30}N_2O_3$ $C_6H_8O_7$	586.63	Not Determined

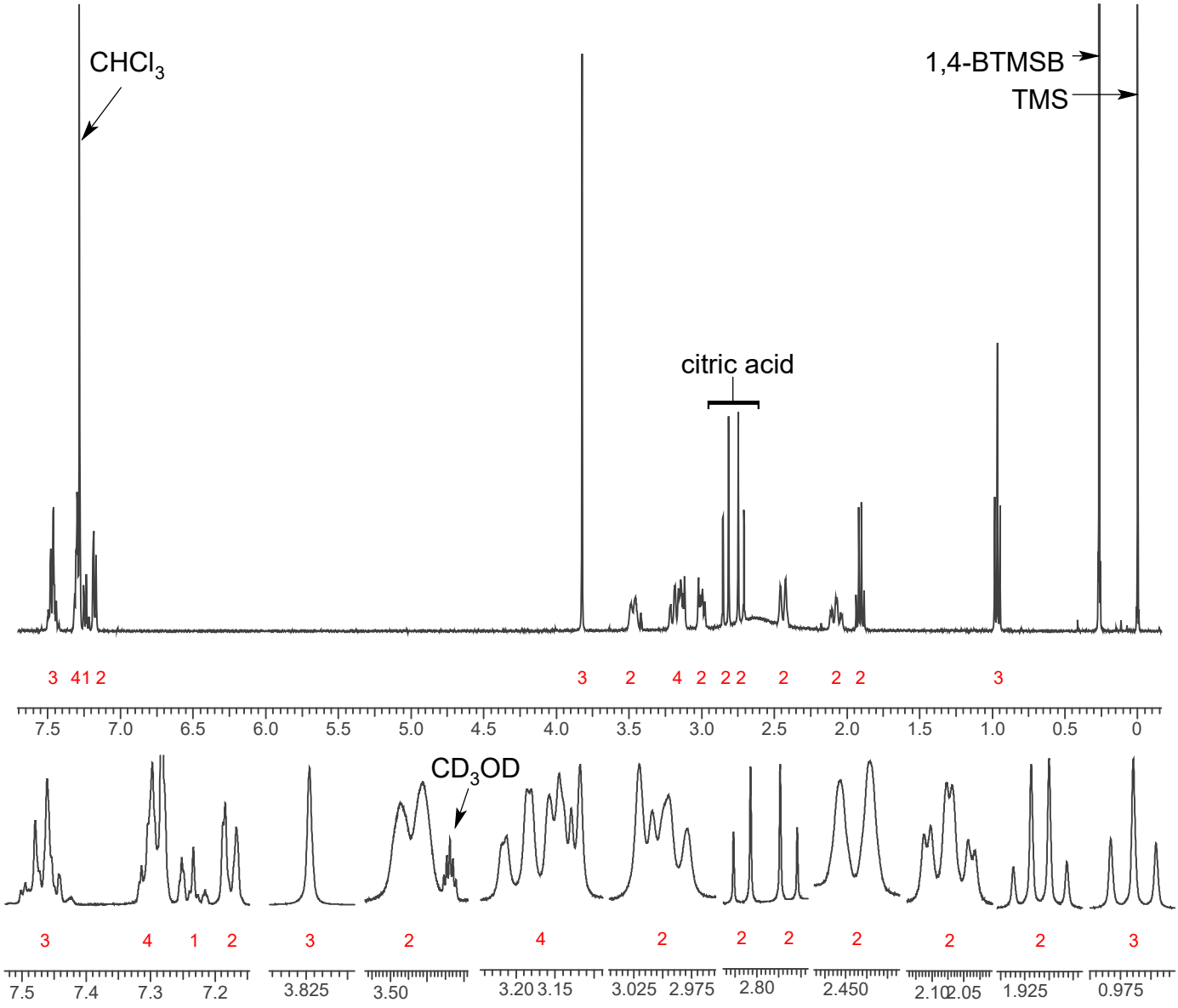
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~5.2 mg/mL in $CDCl_3$ containing TMS for 0 ppm reference and 1,4-BTMSB as quantitative internal standard. One drop of methanol-d_4 added for solubility.

Instrument: 400 MHz NMR spectrometer
Parameters: Spectral width: at least containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds

^{1}HNMR: Carfentanil Citrate Lot# MDM M09047-12; $CDCl_3$; 400MHz

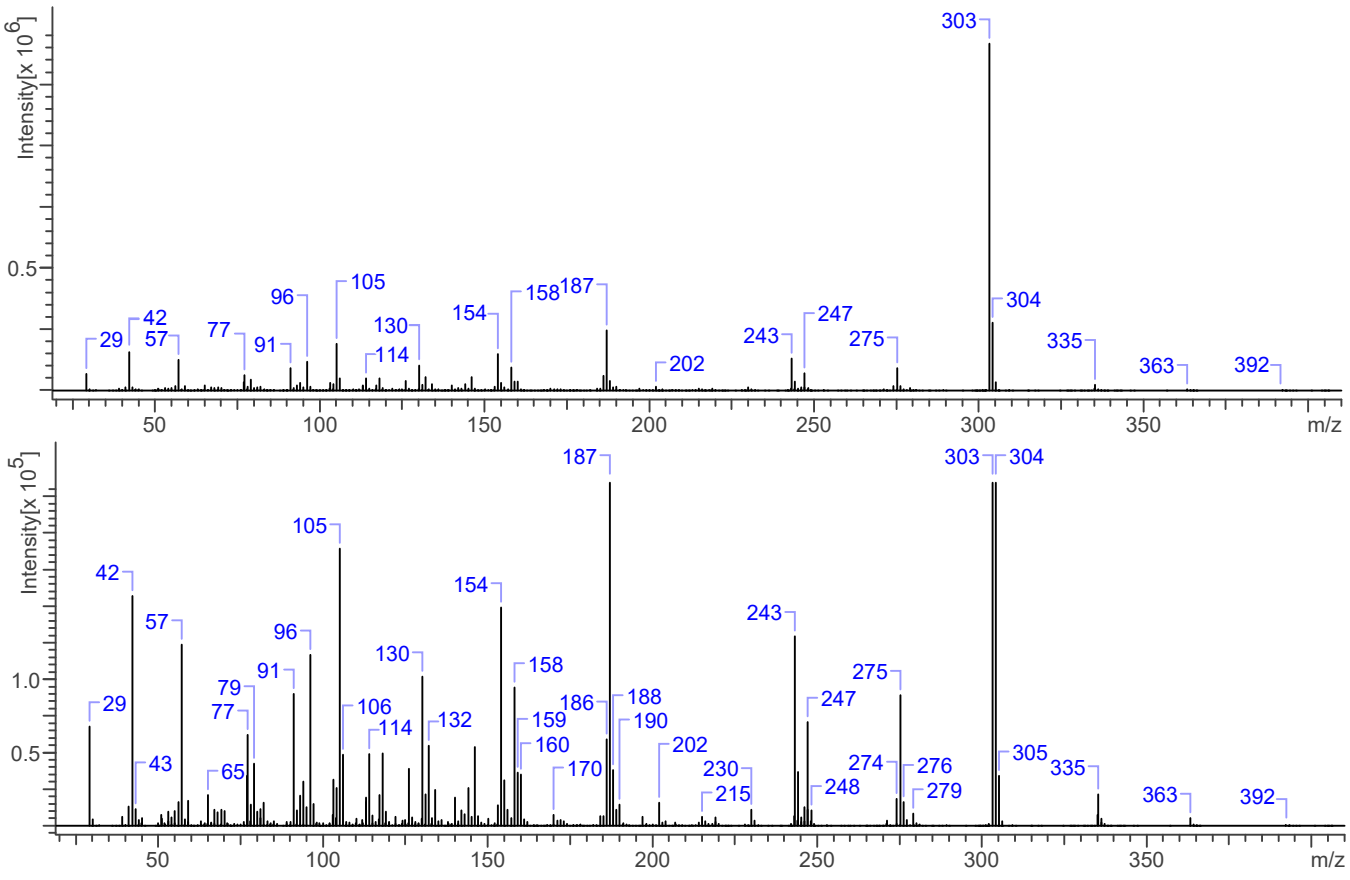


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~2.3 mg/mL in 9:1 $CHCl_3$: 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 µm	
Carrier Gas:	Helium at 1.0 mL/min	
Temperatures:	Injector: 280°C	MSD transfer line: 280°C
	MS Source: 230°C	MS Quad: 150°C
	Oven program:	
	1) 90°C initial temperature for 2.0 min	
	2) Ramp to 300°C at 14 °C/min	
	3) Hold final temperature for 10.0 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:	17.96 min	

EI Mass Spectrum: Carfentanil Citrate Lot# MDM M09047-12

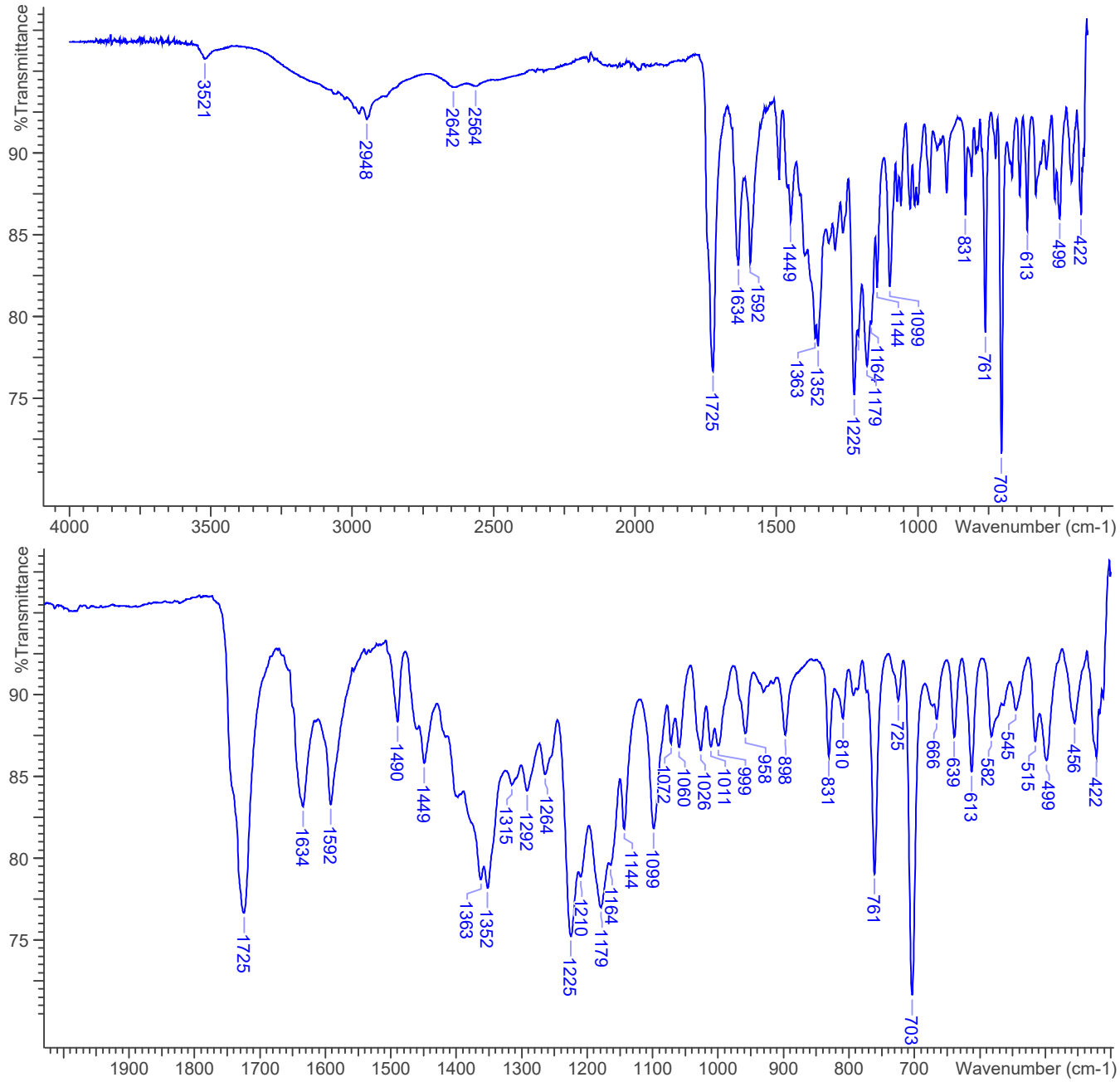


3.3 INFRARED SPECTROSCOPY (FTIR)

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: 80

FTIR ATR (Diamond 1 Bounce): Carfentanil Citrate Lot# MDM M09047-12



4. ADDITIONAL RESOURCES

Wikipedia

Forendex