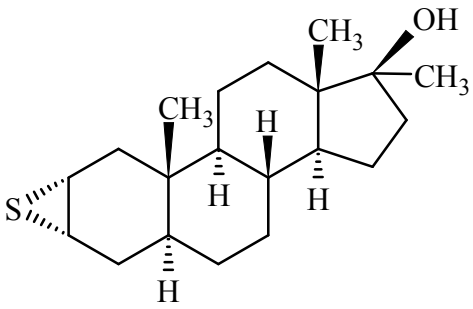
Methylepitiostanol

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



1. GENERAL INFORMATION

IUPAC Name: 2α,3α-epithio-17α-methyl-5α-androstan-17β-ol

CAS#: NA

Synonyms: (2α,3α,5α,17β)-17-methyl-2,3-epithioandrostan-17-ol, methylepithiostanol,17α-methylepithiostanol

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	$C_{20}H_{32}OS$	320.53	NA

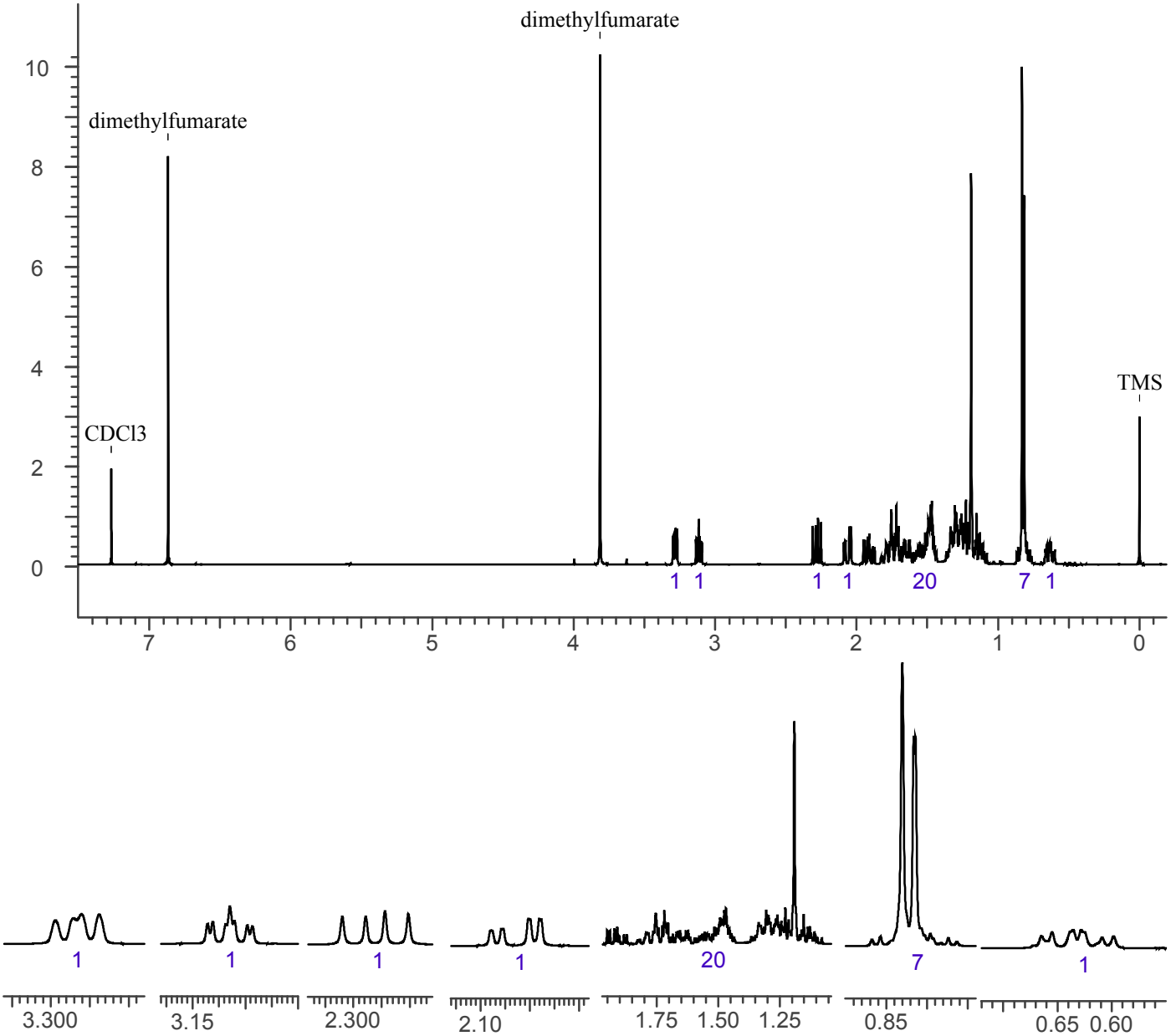
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~18mg/mL in $CDCl_3$ containing TMS for 0 ppm reference and dimethylfumarate 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

^{1}HNMR: Methylepitiostanol Lot#RM-170728-01; $CDCl_3$; 400MHz



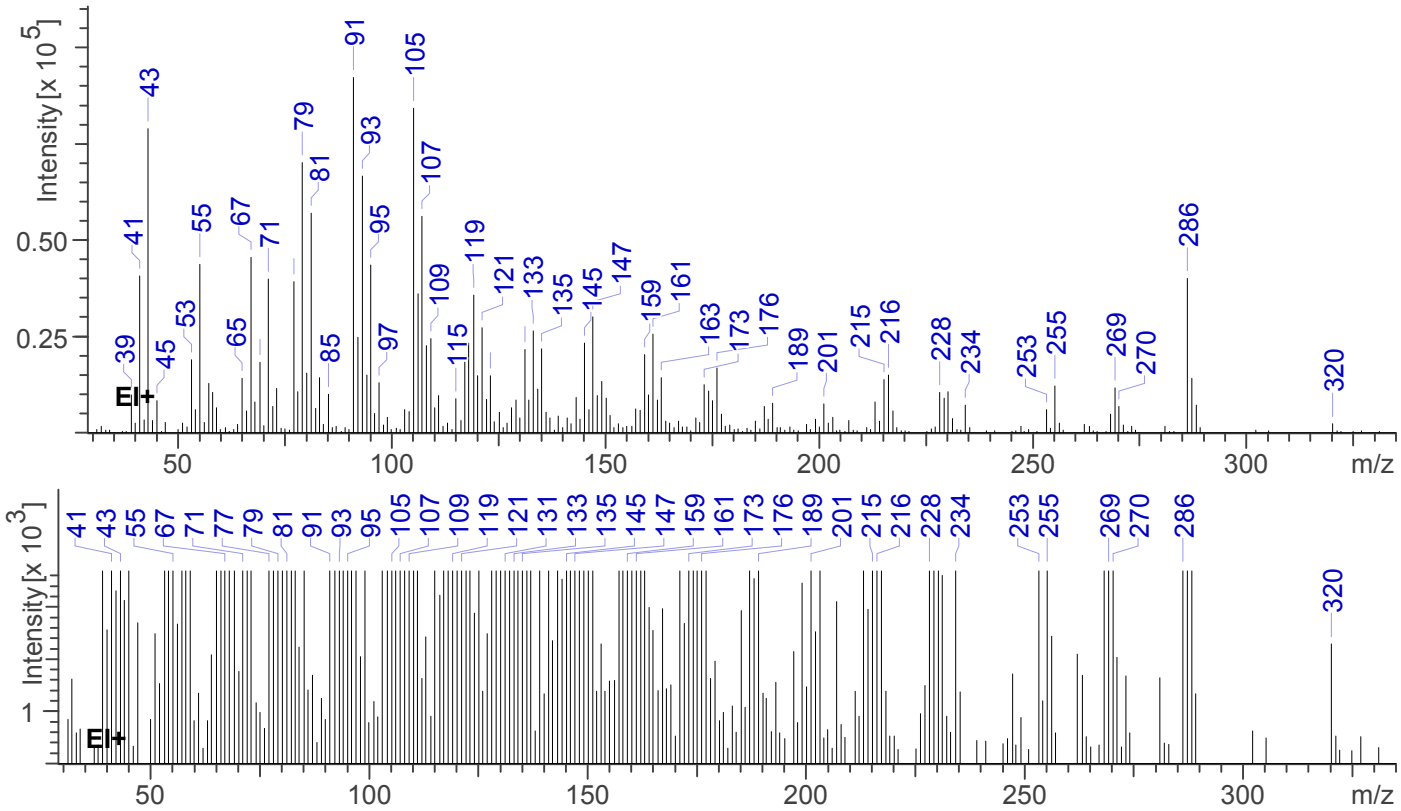
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

*** Methylepitiostanol breaksdown on GC-FID and GC/MS ***

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 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 30.0 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:	17.101 min

EI Mass Spectrum: Methylepitiostanol Lot# RM-170728-01

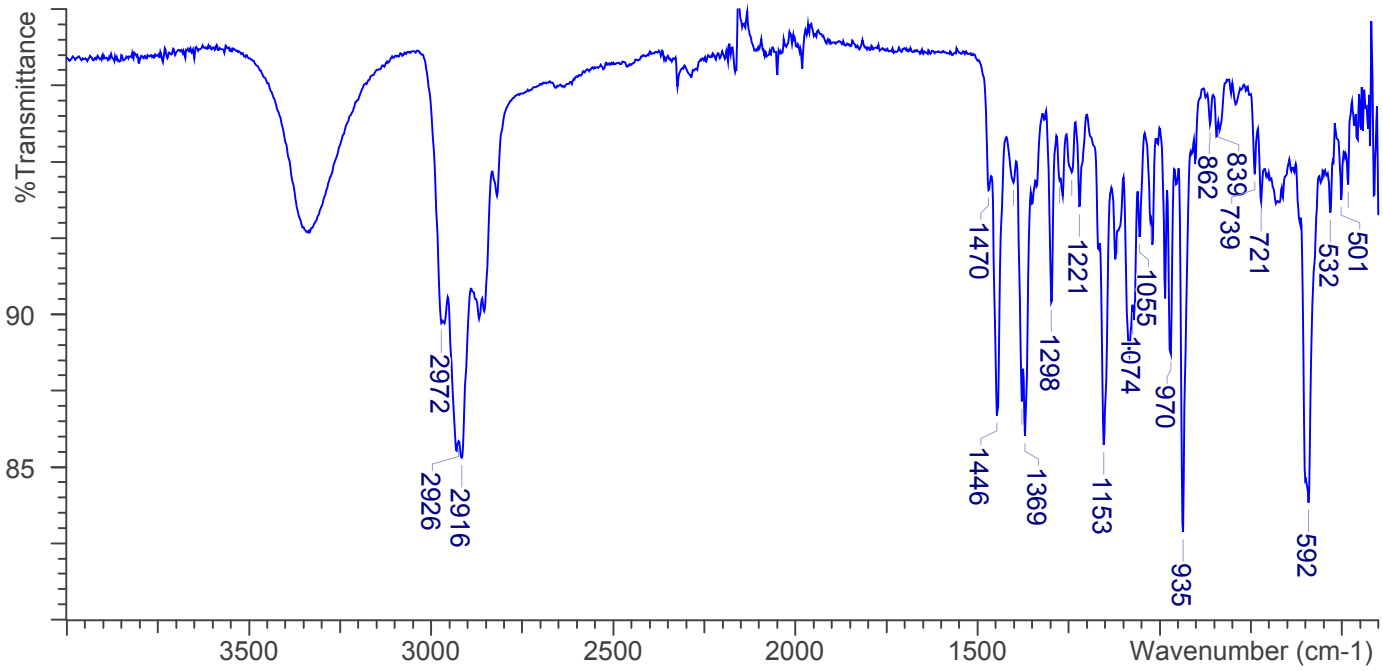


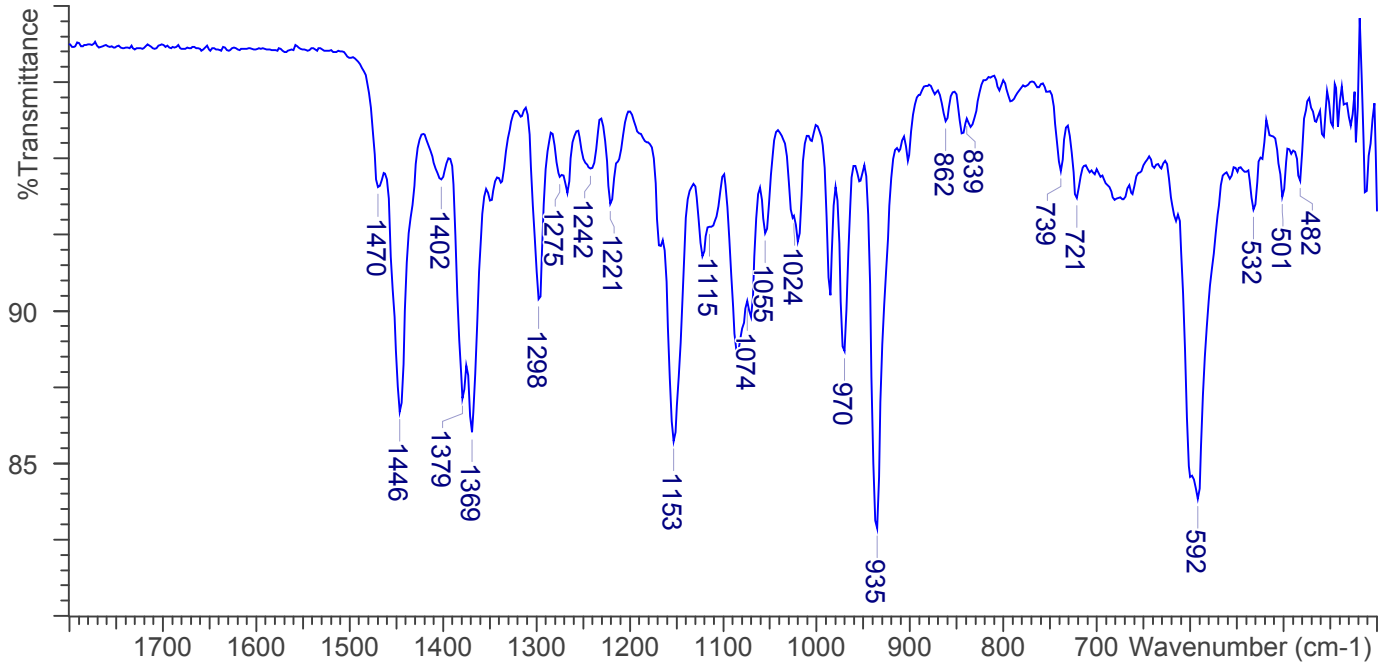
3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR (Smart Golden Gate ATR Accessory)

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): Methylepitiostanol Lot# RM-170728-01





4. ADDITIONAL RESOURCES

Okana, M. et. al., Analysis of non-ketoic steroids 17α-methylepithiostanol and desoxymethyltestosterone in dietary supplements, Drug Test. Analysis 2009, 1, 518-525.