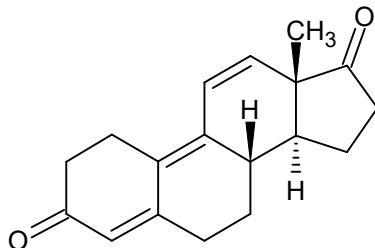




Trendione

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



1. GENERAL INFORMATION

IUPAC Name:	estra-4,9,11-triene-3,17-dione
CAS#:	4642-95-9
Synonyms:	Trenavar
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)
Neutral	C ₁₈ H ₂₀ O ₂	268.35	Not Determined



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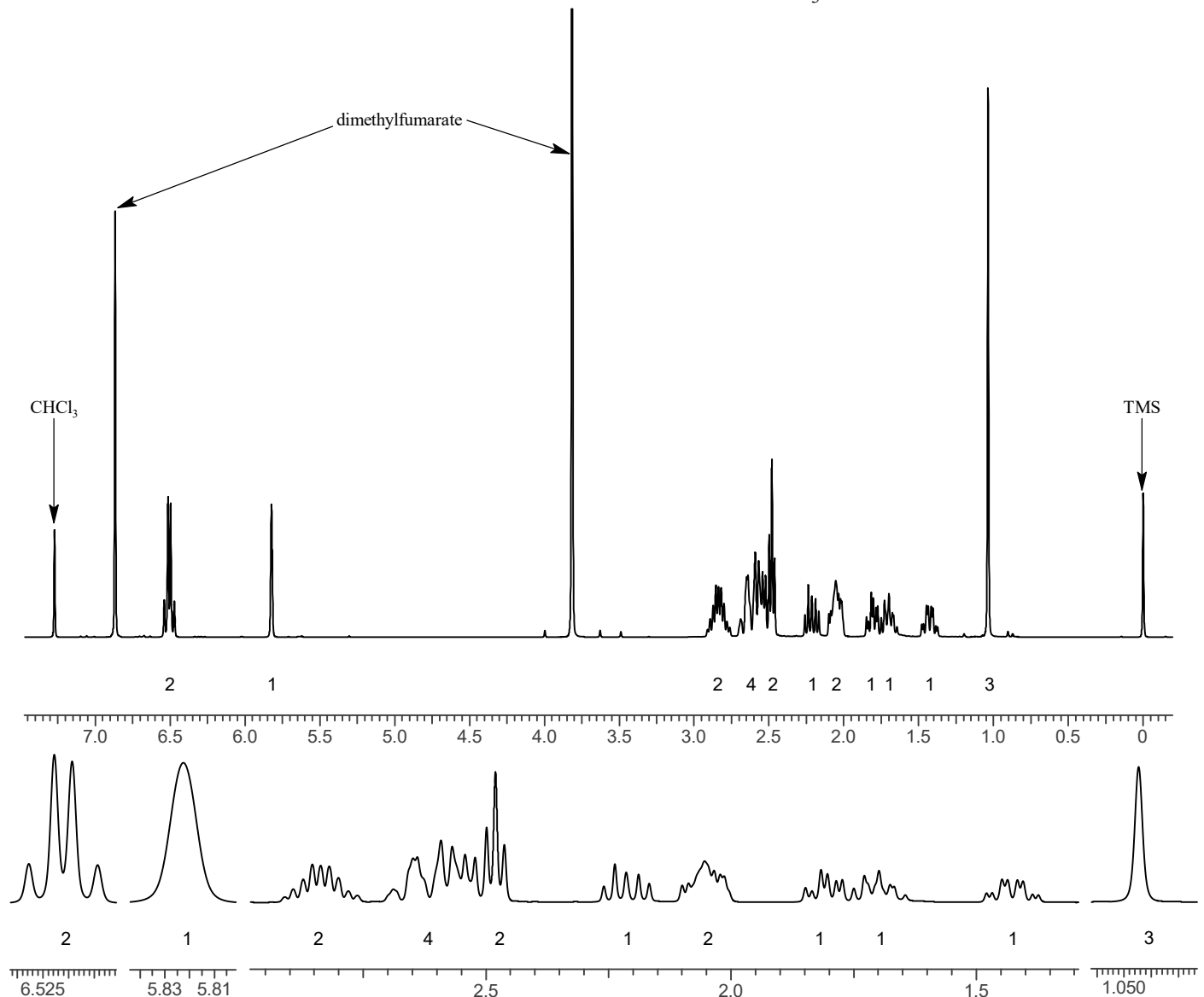
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~10 mg/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

^1H NMR: Trendione; Lot# RM-150319-01; CDCl_3 ; 400MHz





Trendione



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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~6 mg/mL in ether

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

Column: DB-5 MS (or equivalent); 15m 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

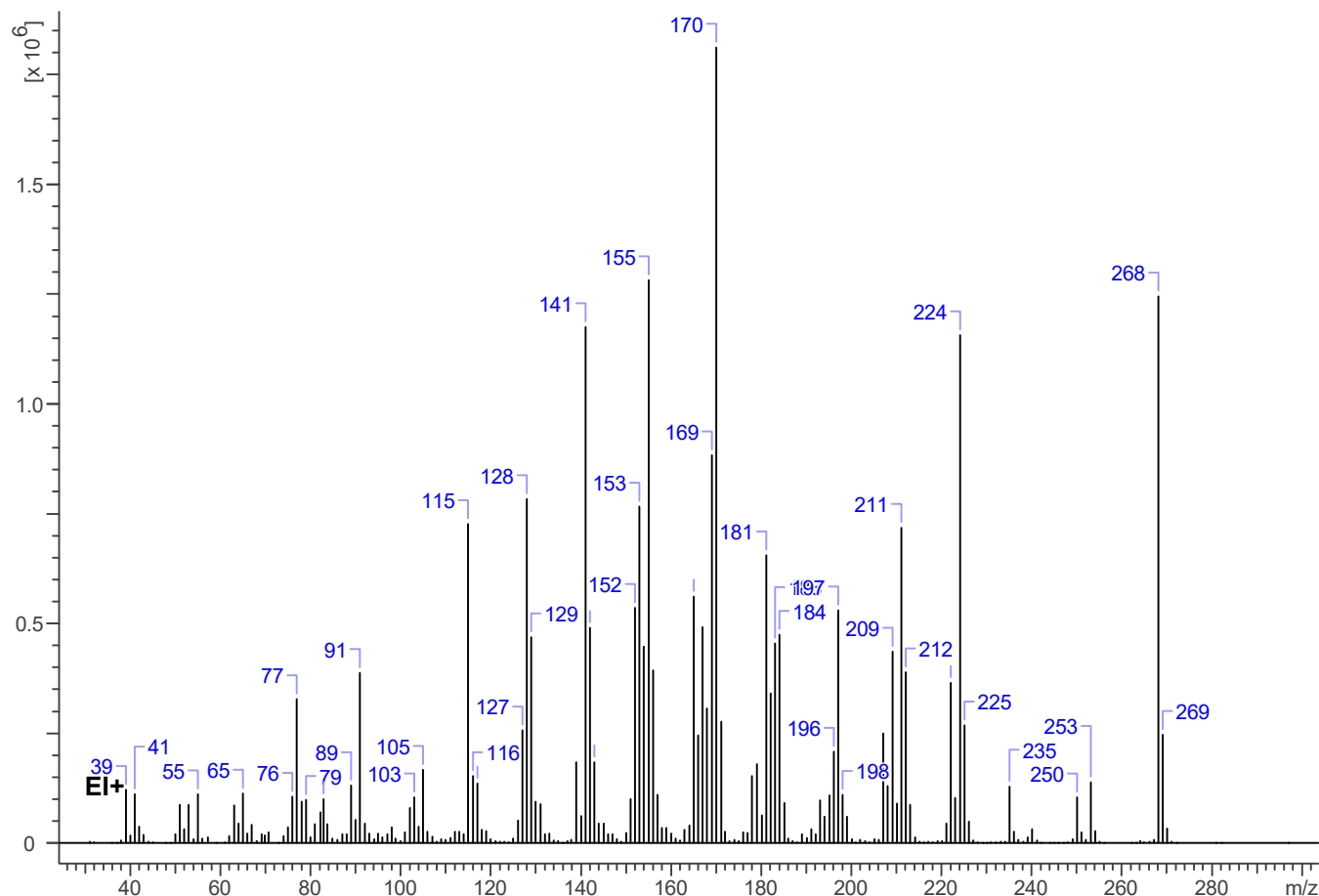
Injection Parameters: Split Ratio = 25:1, 1 μ L injected

MS Parameters: Mass scan range: 30-550 amu Threshold: 150

Tune file: stune.u Acquisition mode: scan

Retention Time: 13.47 min

EI Mass Spectrum: Trendione; Lot# RM-150319-01





Trendione

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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): Trendione; Lot# RM-150319-01

