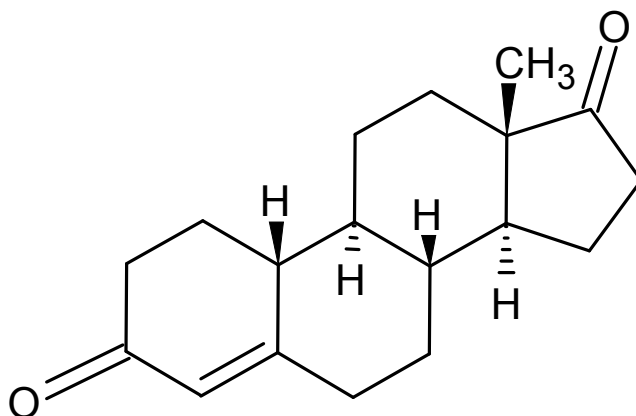




4-estren-3,17-dione

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



1. GENERAL INFORMATION

| | |
|------------------------------|--|
| IUPAC Name: | estr-4-ene-3,17-dione |
| CAS#: | Not Available |
| Synonyms: | 19-nor-4-androsten-3,17-dione; 19-norandrostendione; NOR, bolandione |
| 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) |
|------|--|------------------|--------------------|
| Base | C ₁₈ H ₂₄ O ₂ | 272.38 | 171.4 |



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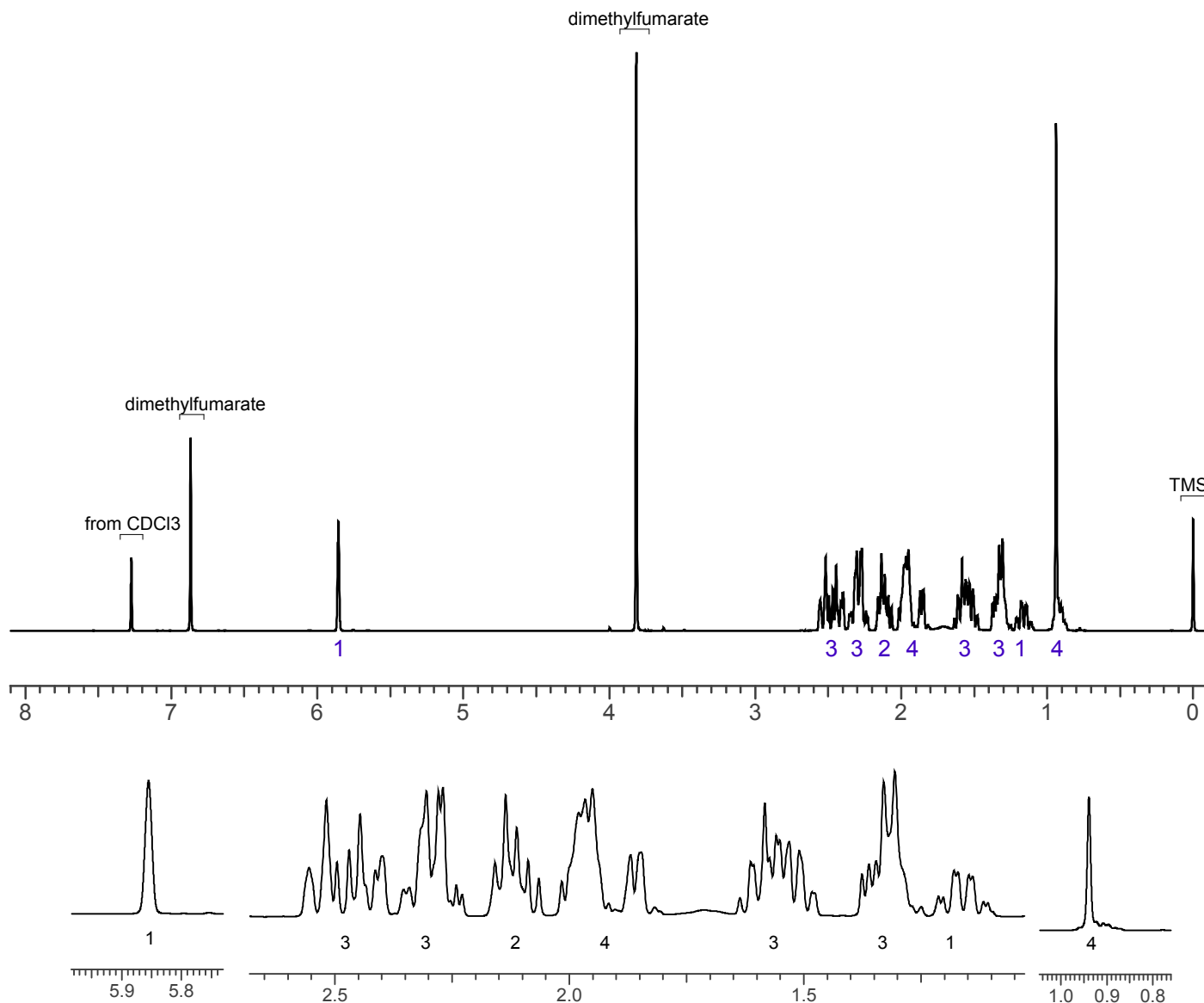


3. QUALITATIVE DATA

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: 4-estren-3,17-dione Lot B1212; CDCl_3 ; 400MHz





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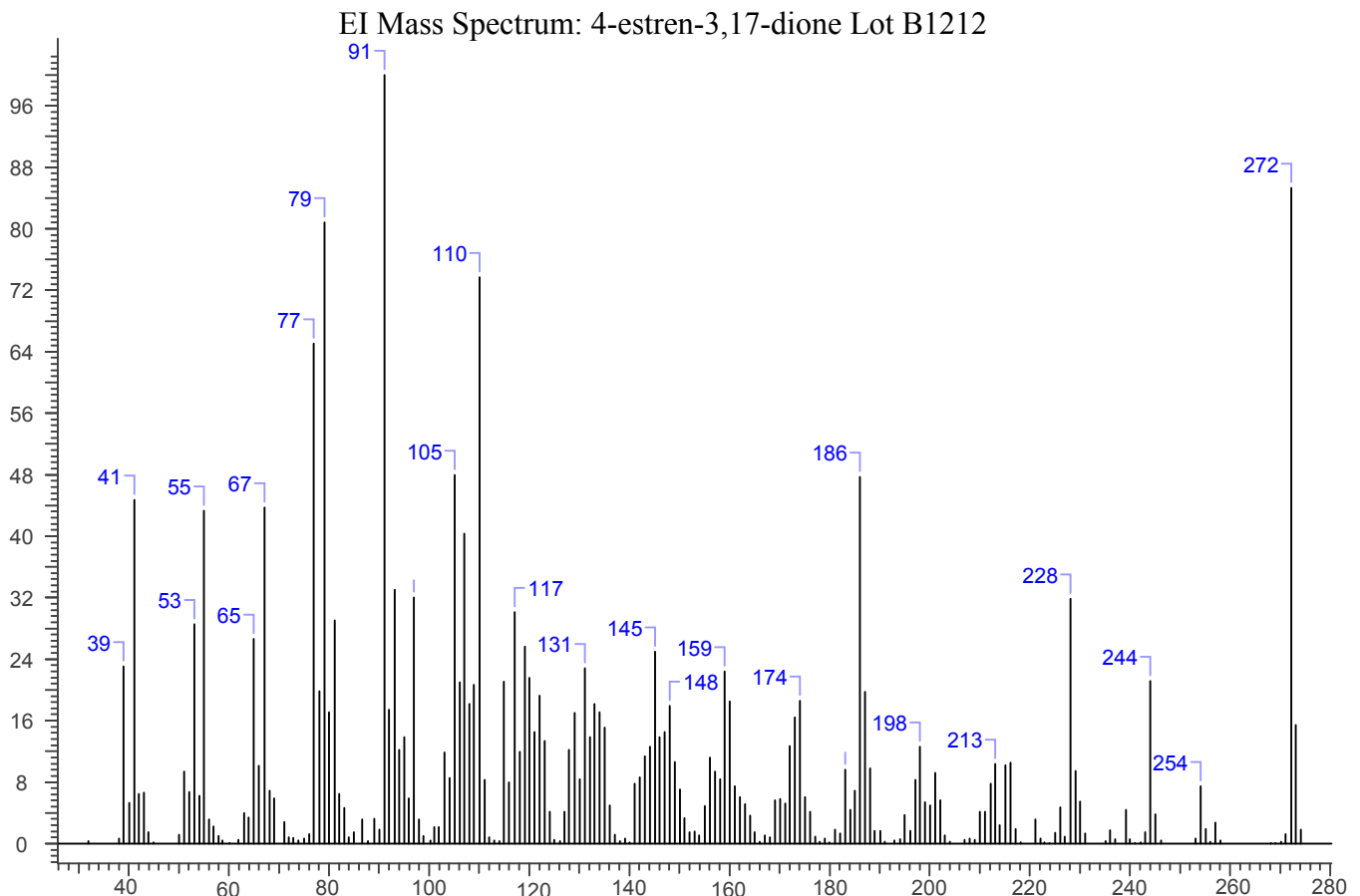
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~2 mg/mL in methanol.

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 μ m
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 9.0 min

Injection Parameters: Split Ratio = 20:1, 1 μ L injected
MS Parameters: Mass scan range: 30-550 amu
Threshold: 100
Tune file: stune.u
Acquisition mode: scan

Retention Time: 14.926 min





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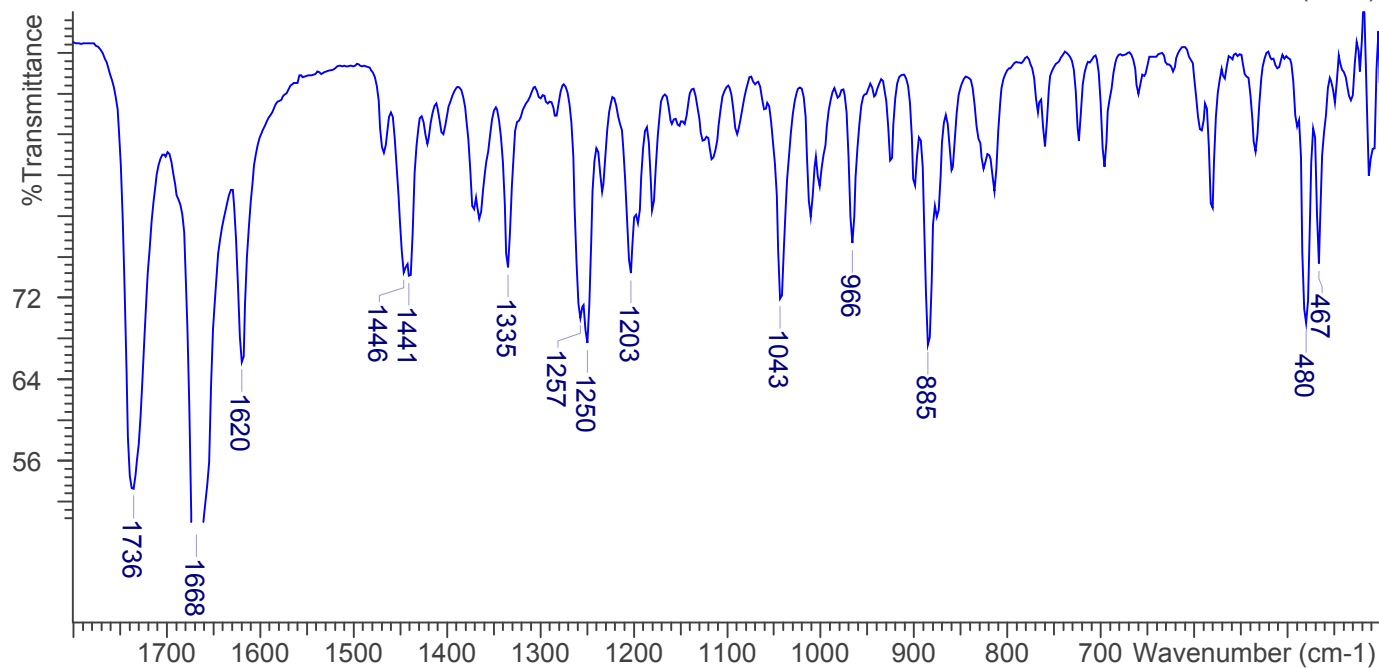
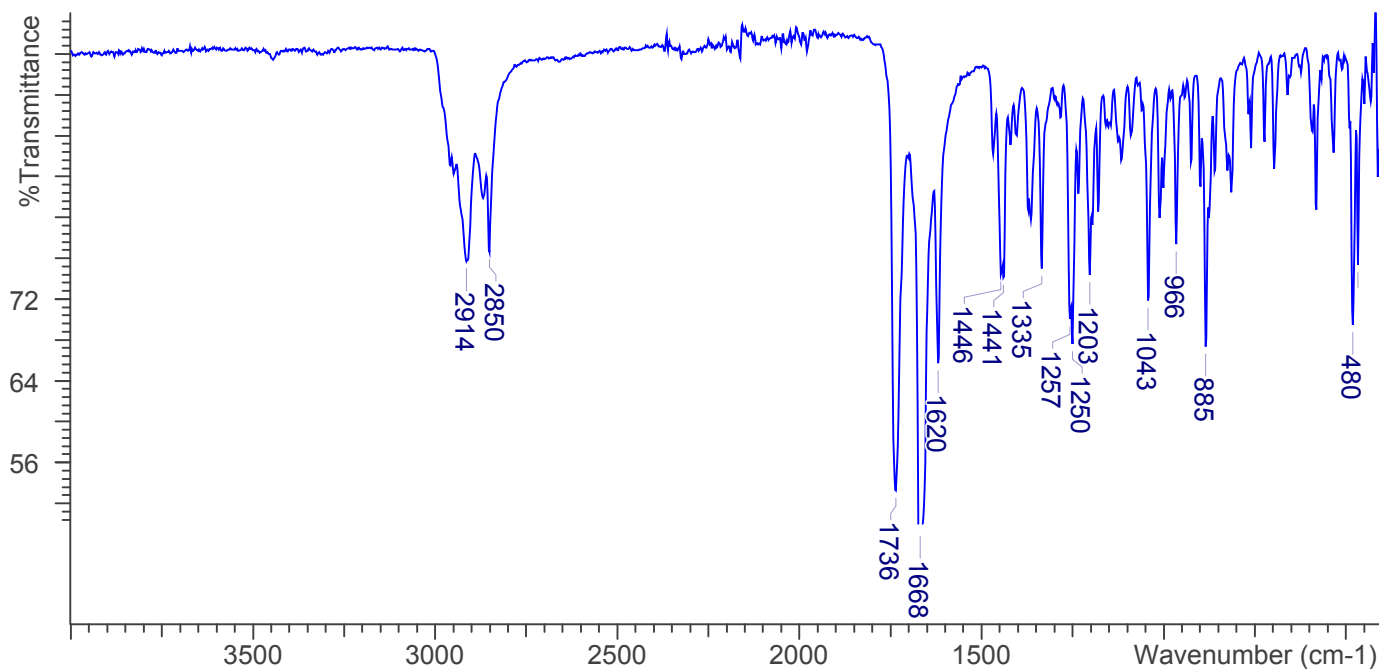


3.3 INFRARED SPECTROSCOPY (FTIR)

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): 4-estren-3,17-dione Lot B1212





4-estren-3,17-dione

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4. ADDITIONAL RESOURCES

[Forendex](#)

[Wikipedia](#)