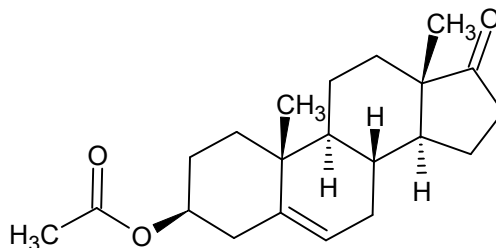




Dehydroisoandrosterone 3-Acetate

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



1. GENERAL INFORMATION

IUPAC Name:	17-oxoandrost-5-en-3 β -yl acetate
CAS#:	853-23-6
Synonyms:	Dehydroepiandrosterone 3-acetate, 3- β -Acetoxy-5-androsten-17-one, 5-androsten-3 β -ol-17-one acetate, 5-dehydroisoandrosterone-3-acetate
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 (g/mol)	Melting Point (°C)
Base	C ₂₁ H ₃₀ O ₃	330.46	168.09



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3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~24 mg/mL in CD₃OD containing TMS for 0 ppm reference and maleic acid as quantitative internal standard.

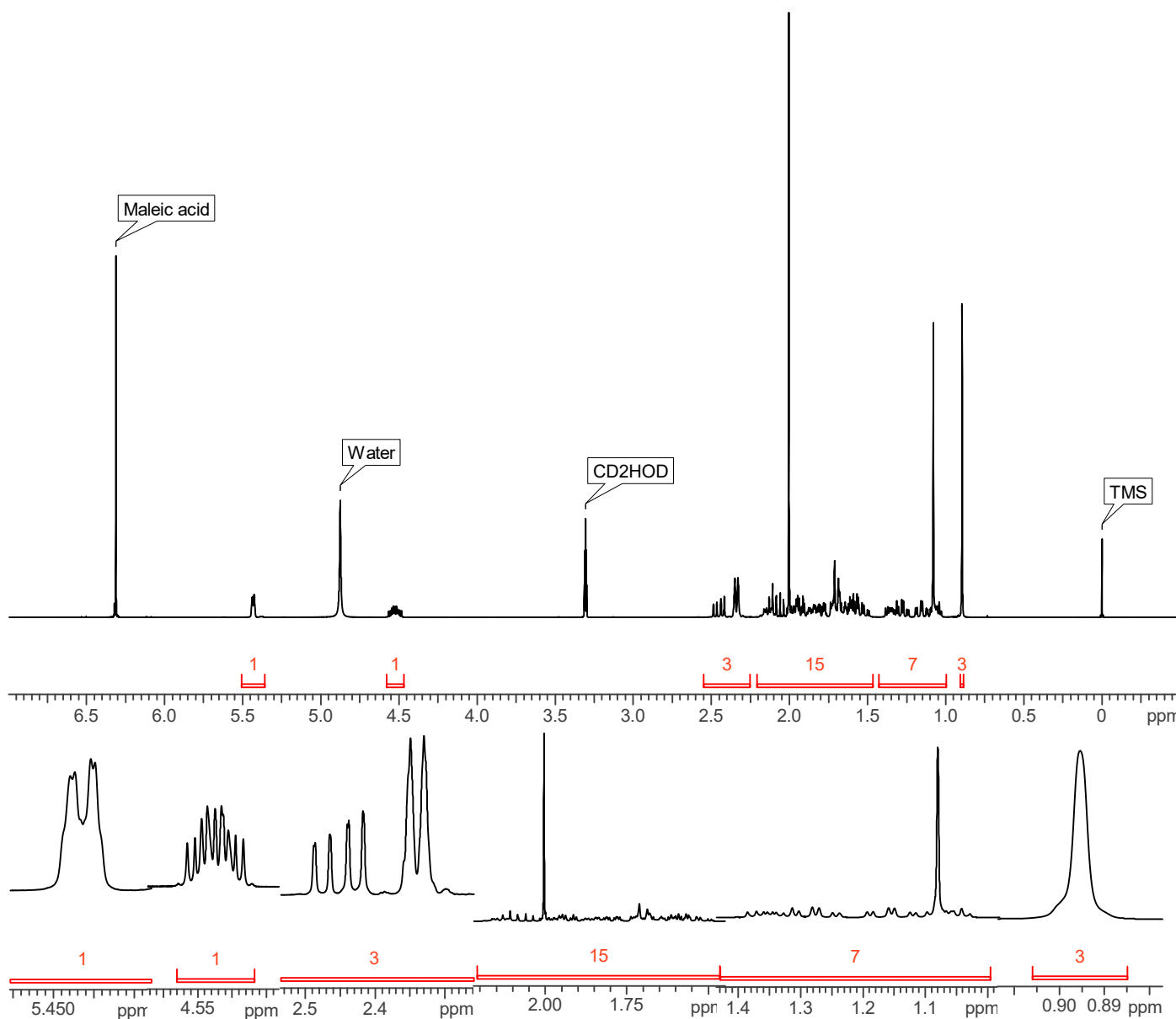
Instrument: 400 MHz NMR spectrometer

Parameters: Spectral width: at least containing -3 ppm through 13 ppm

Pulse angle: 90°

Delay between pulses: 45 seconds

¹HNMR: Dehydroisoandrosterone 3-Acetate; Lot# 17984; CD₃OD; 400 MHz





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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

Instrument: Agilent gas chromatograph operated in split mode with MS detector
Column: HP-5 MS (or equivalent); 30 m 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

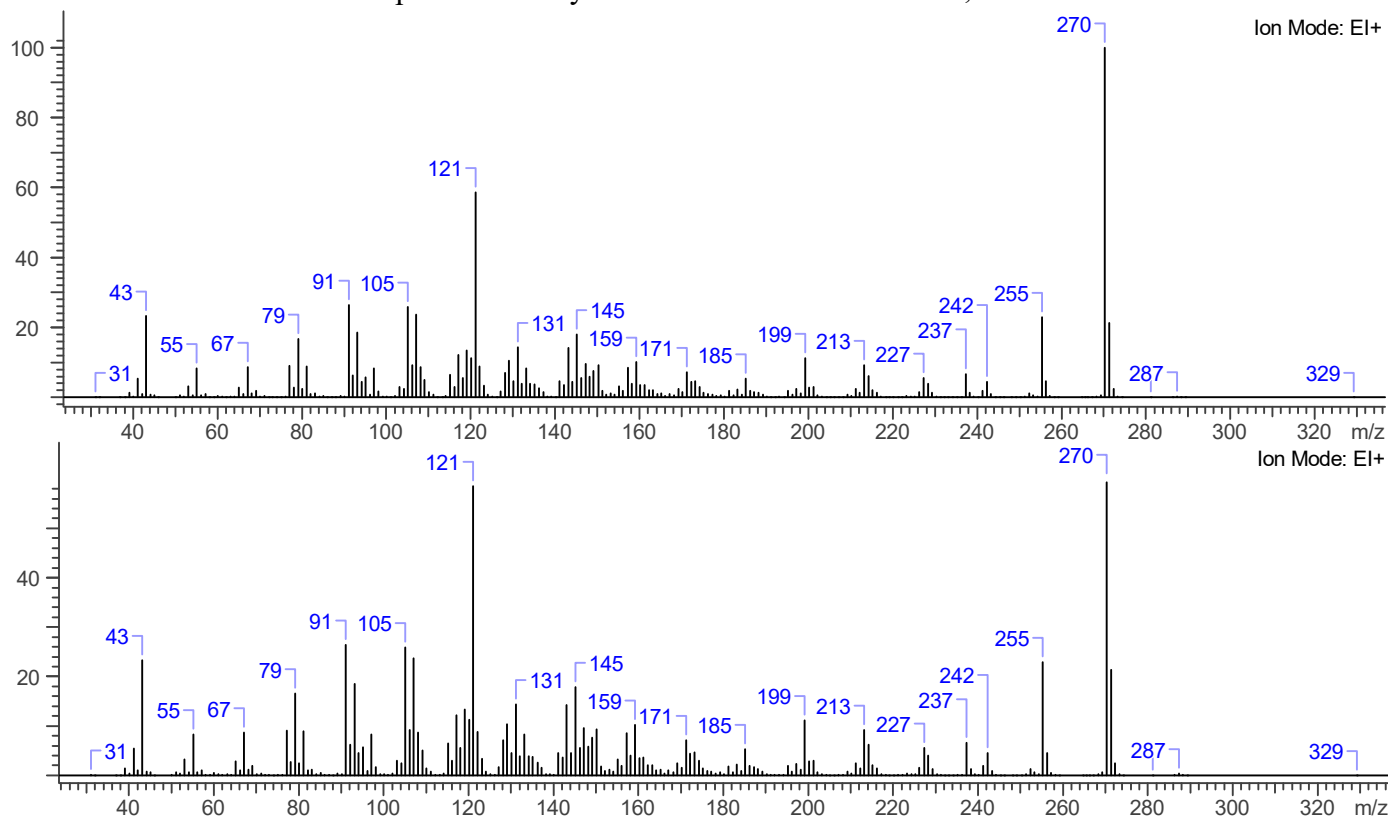
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

Retention Time: 15.797 min

EI Mass Spectrum: Dehydroisoandrosterone 3-Acetate; Lot# 17984





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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: 4
Aperture: 150

FTIR ATR (Diamond 1 Bounce): Dehydroisoandrosterone 3-Acetate; Lot#17984

