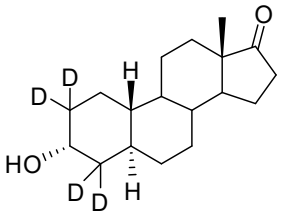
DEUTERATED INTERNAL STANDARD PRODUCT INFORMATION SHEET

NMIA D584c: d4-19-Norandrosterone

Report ID: D584c.2026.01

Chemical Formula: $C_{18}H_{24}D_4O_2$

Molecular Weight: 280.4 g/mol



Property value

Batch No.	CAS No.	Purity estimate
13-S-09	361432-47-5	93.0 ± 2.2%

The uncertainty has been calculated according to ISO 33405 and is stated at the 95% confidence limit (k = 2).

IUPAC name: (3α,5α)-3-Hydroxy(2,2,4,4-$^2H_4$)estran-17-one.

Expiration of certification: The property values are valid till 24 July 2036, ten years from the date of re-certification provided the **unopened** material is handled and stored in accordance with the recommendations below. The material as issued in the unopened container and stored as recommended below should be suitable for use beyond this date, subject to confirmation of batch stability from the issuing body. The expiry date/shelf life does not apply to sample bottles that have been opened. In such cases it is recommended that the end-user conduct their own in-house stability trials. The material will be re-tested periodically to ensure that the property values are still valid. In the event a product fails the stability trial, notification will be sent to all impacted customers.

Description: White crystalline solid prepared by synthesis and certified for identity and purity by NMI Australia. Packaged in amber glass bottles with a septum and crimped aluminium cap or screw top cap.

Intended use: The isotopic purity of this material is an estimate only. This material should be considered for use as an internal standard only.

Instructions for use: Equilibrate the bottled material to room temperature before opening.

Recommended storage: When not in use this material should be stored at or below 4 ºC in a closed container in a dry, dark area.

Stability: The long-term stability of the compound in solution has not been examined.

Homogeneity assessment: The homogeneity of the material was assessed using purity assay by GC-FID on seven randomly selected 1-2 mg sub samples of the material. The material was judged to be sufficiently homogeneous at this level of sampling as the variation in analysis results between samples was not significantly different at a 95% confidence level from that observed on repeat analysis of the same sample.

Safety: Treat as a hazardous substance. Use appropriate work practices when handling to avoid skin or eye contact, ingestion or inhalation of dust. Refer to the provided safety data sheet.

S. R. Davies

Dr Stephen R. Davies,
Team Leader,
Chemical Reference Materials, NMI.
4 August 2026

This report supersedes any issued prior to 04 August 2026.

NATA Accreditation No. 198 / Corporate Site No. 14214.

Characterisation Report:

The identity was confirmed by a range of spectroscopic techniques, NMR, IR and MS. The indicative purity value was obtained by mass balance from a combination of traditional analytical techniques, including GC-FID, thermogravimetric analysis, Karl Fischer analysis, and ^{1}H NMR spectroscopy. The purity value is calculated as per Equation 1.

Purity = (100 % - I_{ORG}) x (100 % - I_{VOL} – I_{NVR}) Equation 1

I_{ORG} = Organic impurities of related structure, I_{VOL} = volatile impurities, I_{NVR} = non-volatile residue.

Supporting evidence is provided by qualitative elemental microanalysis.

The main component of this material is d_4-19-norandrosterone. d_3-, d_2-, d_1- and d_0-19-Norandrosterone are also present. The stated chemical purity of the analyte represents the combined mass fractions of deuterated (d_4, d_3, d_2 and d_1) and d_0-19-norandrosterone in the material.

The isotopic purity of this material is an estimate only. This material should be considered for use as an internal standard only.

Isotopic Purity: $d_4 \approx 90\%$ [= $d_4/(d_4 + d_3 + d_2 + d_1 + d_0) \times 100$]

$d_0 < 0.2\%$ [= $d_0/(d_4 + d_3 + d_2 + d_1 + d_0) \times 100$]

GC-FID:

Instrument:	Agilent 6890 or Agilent 8890	
Column:	HP-1MS, 30 m × 0.32 mm I.D. × 0.25 µm	
Program:	200 °C (13 min), 20 °C/min to 300 °C (3 min)	
Injector:	250 °C	Detector Temp: 320 °C
Carrier:	Helium	Split ratio: 20/1

Relative peak area of main component:

Initial analysis:	Mean = 99.1%, s= 0.04% (10 sub samples in duplicate, October 2013)
Re-analysis:	Mean = 99.5%, s = 0.52% (7 sub samples in duplicate, August 2025)
	Mean = 99.5%, s = 0.04% (5 sub samples in duplicate, July 2026)

Karl Fischer analysis:
Moisture content ≤ 0.1% mass fraction (October 2013)
Moisture content 6.0% mass fraction (August 2025, July 2026)

Thermogravimetric analysis:
Non volatile residue < 0.2% mass fraction (October 2013). The volatile content (e.g. organic solvents and/or water) could not be determined because of the inherent volatility of the material and/or degradation at elevated temperatures.

Non volatile residue was re-analysed (August 2025) and showed < 0.1%. The volatile content (e.g. organic solvents and/or water) could not be determined because of the inherent volatility of the material and/or degradation at elevated temperatures.

Spectroscopic and other characterisation data

GC-MS:

Parent compound:

Instrument:	Agilent 6890/5973	
Column:	TG1-MS, 30 m x 0.25 mm I.D. x 0.25 μm	
Program:	180 °C (1 min), 10 °C/min to 300 °C (3 min)	
Injector:	250 °C	Transfer line temp: 280 °C
Carrier:	Helium, 1.0 mL/min	Split ratio: 20/1

Bis-TMS derivative:

Instrument:	Agilent 6890/5973	
Column:	TG1-MS, 30 m x 0.25 mm I.D. x 0.25 μm	
Program:	180 °C (1 min), 10 °C/min to 300 °C (3 min)	
Injector:	250 °C	Transfer line temp: 280 °C
Carrier:	Helium, 1.0 mL/min	Split ratio: 20/1

The retention times of the parent compound and *bis*-TMS derivative are reported along with the major peaks in the mass spectra. The latter are reported as mass/charge ratios and (in brackets) as a percentage relative to the base peak.

Parent (9.2 min): 280 (M^+, 100), 262 (22), 236 (36), 218 (19), 206 (51), 191 (29), 163 (20), 151 (27), 135 (18), 124 (20), 108 (21), 97 (26), 92 (31), 79 (31), 67 (30) *m/z*

Bis-TMS (9.9 min): 424 (M^+, 64), 409 (100), 337 (12), 319 (24), 229 (14), 169 (33), 73 (100) *m/z*
The silylated compound co-elutes with a derivatised comparison sample of norandrosterone

TLC:
Conditions: Kieselgel 60F_{254}. Chloroform/ethyl acetate (4/1)
Single spot observed, R_f = 0.6 Visualisation with vanillin

IR:
Instrument: FT-IR, Biorad WIN FTS40
Range: 4000-400 cm^{-1}, KBr pellet
Peaks: 3479, 1723, 1443, 1091 cm^{-1}

^{1}H NMR:
Instrument: Bruker Avance III-400
Field strength: 400 MHz
Solvent: $CDCl_3$ (7.26 ppm)
Spectral data: δ 0.68-0.82 (2H, m), 0.86 (3H, s), 0.96-1.44 (9H, m), 1.49 (1H, m), 1.58-1.62 (1H, m), 1.69 (1H, dd, *J* = 3.1, 13.4 Hz), 1.74-1.80 (2H, m), 1.84-1.95 (2H, m), 2.06 (1H, dt, *J* =19.2, 9.0 Hz), 2.43 (1H, ddd, *J* = 0.7, 8.7, 19.1 Hz), 4.07 (1H, d, *J* = 2.4 Hz) ppm
Ethyl acetate estimated at 0.6% mass fraction was observed in the ^{1}H NMR

^{13}C NMR:
Instrument: Bruker DMX-500
Field strength: 126 MHz
Solvent: $CDCl_3$ (77.19)
Spectral data: δ 14.0, 21.8, 23.7, 25.1, 30.0, 31.8, 32.4 (m), 33.6, 36.0, 39.9 (m), 41.0, 47.1, 48.1, 48.5, 50.9, 66.3, 221.6 ppm.

Melting point: 164-166 °C

Microanalysis:
Found: C = 76.6%; H+D = 10.3% (November 2013)
Calculated: C = 77.1%; H+D = 10.0% (Calculated for $C_{18}H_{24}D_4O_2$)