Australian Government
Department of Industry, Science and Resources

National Measurement Institute

NATA
WORLD RECOGNISED ACCREDITATION

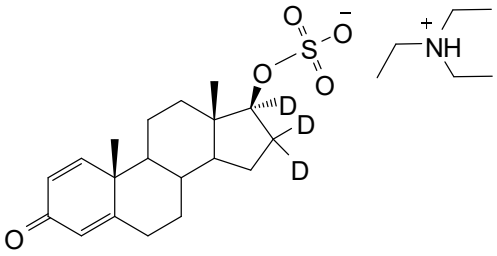
DEUTERATED INTERNAL STANDARD PRODUCT INFORMATION SHEET

NMIA S013: d_3-Boldenone sulfate triethylamine salt

Report ID: S013.2026.02 (Ampouled 121015)

Chemical Formula: $C_{25}H_{38}D_3NO_5S$

Molecular Weight: 470.7 g/mol



Property value

Batch No.	CAS No.	Mass per ampoule
11-S-12	Not available	897 ± 21 µg

Synonyms: 17β-(Sulfoxy)-androsta-1,4-dien-3-one-16,16,17-d_3 triethylamine salt.

Expiration of certification: The property values are valid till 30 January 2029, three 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 shelf life does not apply to ampoules that have been opened. In such cases it is recommended that the end-user conduct their own in-house stability trials.

Description: The compound is supplied as a dried aliquot in a sealed ampoule and is intended for a single use to prepare a standard solution containing S013. The material was prepared by synthesis and certified for identity and purity by NMI Australia.

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: Open the ampoule and carefully rinse the interior at least three times with a suitable organic solvent (e.g. methanol). This will transfer approximately 897 ± 21 µg of anhydrous boldenone sulfate triethylamine salt (d_3, d_2, d_1 and d_0).

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: This material has demonstrated stability over a minimum period of three years. 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 HPLC with UV detection on seven randomly selected ampoules 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.
6 February 2026.

This report supersedes any issued prior to 6 February 2026.

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

Legal notice: Terms and Conditions associated with the provision of this reference material can be found on the NMIA website.

Characterisation Report:

HPLC:	Instrument:	Waters Model 1525 Binary pump, 717 plus auto sampler or Shimadzu Binary pump LC-20AB, SIL-20 A HT auto sampler
	Column:	X-Bridge C-18, 5 μm (4.6 mm × 150 mm)
	Column oven:	40 °C
	Mobile Phase:	Milli-Q water/Methanol A = Milli-Q water; B = Methanol 0.05%TFA was present in both aqueous and organic phase 0-14 min 44% B; 14-18 min 44-80% B; 18-22 min 80% B; 22-23 min 80-44% B, 23-30 min 44 % B
	Flow rate:	1.0 mL/min
	Detector:	Shimadzu SPD-M20A or Waters 2998 PDA operating at Max plot.
	Relative peak area of the main component:	
	Initial analysis:	Mean = 93.0%, s = 0.18% (7 ampoules in duplicate, October 2012)
	Re-analysis:	Mean = 93.2%, s = 0.04% (5 ampoules in duplicate, September 2013)
	Re-analysis:	Mean = 93.2%, s = 0.04% (5 ampoules in duplicate, August 2016)
	Re-analysis:	Mean = 93.1%, s = 0.04% (5 ampoules in duplicate, July 2019)
	Re-analysis:	Mean = 93.3%, s = 0.05% (5 ampoules in duplicate, February 2022)
	Re-analysis:	Mean = 93.6%, s = 0.15% (5 ampoules in duplicate, January 2026)

The following analytical data was obtained on the bulk material subsequently used in the preparation of the ampoules.

The identity was confirmed by a range of spectroscopic techniques, NMR, IR and MS. The purity value was obtained by mass balance from a combination of traditional analytical techniques, including HPLC with UV, 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_3-boldenone sulfate triethylamine salt. d_3-, d_2-, d_1- and d_0-Boldenone sulfate triethylamine salt are also present. The stated mass of the analyte per ampoule represents the combined masses of deuterated (d_3, d_2 and d_1) and d_0-boldenone sulfate triethylamine salt 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_3 ≈ 97% [= $d_3/(d_3 + d_2 + d_1 + d_0)$ x 100] d_0 < 0.5% [= $d_0/(d_3 + d_2 + d_1 + d_0)$ x 100] [from SIM analysis of the free steroid]
HPLC:	Instrument:	Shimadzu Binary pump LC-20AB, SIL-20 A HT auto sampler
	Column:	X-Bridge C-18, 5 μm (4.6 mm × 150 mm)
	Column oven:	40 °C
	Mobile Phase:	Methanol/Milli-Q water (44:56 v/v)
	Flow rate:	1.0 mL/min
	Detector:	Shimadzu SPD-M20A PDA 2998 operating at Max plot
	Relative peak area of the main component:	
	Initial analysis:	Mean = 93.0%, s = 0.2% (9 sub samples in duplicate, January 2011)
Karl Fischer analysis:		Moisture content 4.4% mass fraction (December 2011)
Thermogravimetric analysis:		Non volatile residue < 0.2% mass fraction. The volatile content (e.g. organic solvents and/or water) could not be determined because of the inherent volatility of the material (December 2011).

Spectroscopic and other characterisation data:

LC-MS:	Instrument:	Waters 2695 (HPLC)/Micromass Quatro
	Ionisation mode:	Electrospray negative ion
	Capillary voltage:	3.0 kV
	Cone voltage:	20 V
	Source temp:	130 ºC
	Desolvation gas temp:	350 ºC
	Cone gas flow rate:	23 L/hr
	Desolvation gas flow:	759 L/hr
	Dissociated Peak:	368.0 (M-triethylamine+) *m/z*
IR:	Instrument:	Biorad FTS3000MX FT-IR
	Range:	4000-400 cm^{-1}, KBr powder
	Peaks:	3354, 3031, 2976, 2940, 2739, 2677, 2491, 2236, 1658, 1620, 1471, 1446, 1260, 1217, 1015, 980, 821 cm^{-1}
^{1}H NMR:	Instrument:	Bruker Avance III-400
	Field strength:	400 MHz
	Solvent:	MeOH-d_4 (3.31 ppm)
	Spectral data:	δ 0.90 (3H, s), 0.93-1.11 (3H, m), 1.29 (3H, s), 1.32 (9H, t, *J* = 7.3 Hz), 1.13-1.49 (2H, m), 1.63 (1H, dd, *J* = 7.2, 12.3 Hz), 1.68-1.85 (3H, m), 1.98-2.05 (2H, m), 2.4 (1H, ddd, *J* = 2.7, 3.8, 13.1 Hz), 2.57 (1H, ddt, *J* = 1.2, 5.2, 20.2 Hz), 3.22 (6H, q, *J* = 7.3 Hz), 6.06 (1H, s), 6.21 (1H, dd, *J* = 1.9, 10.1 Hz), 7.30 (1H, d, *J* = 10.1 Hz) ppm
^{13}C NMR:	Instrument:	Bruker Avance III-400
	Field strength:	100 MHz
	Solvent:	MeOH-d_4 (49.00 ppm)
	Spectral data:	δ 9.2, 12.1, 19.1, 23.6, 24.2, 33.8, 34.5, 36.6, 37.6, 44.0, 45.4, 48.0, 50.9, 54.2, 124.0, 127.5, 159.6, 173.5, 188.7 ppm
Melting point:		97-101°C
Microanalysis:	Found:	C = 61.4%; H = 9.0%; N = 2.9% (November, 2011)
	Calculated:	C = 63.8%; H = 9.4%; N = 3.0% (Calculated for $C_{25}H_{38}D_3NO_5S$)
	Calculated:	C = 61.0%; H = 9.0%; N = 2.9% (Calculated for $C_{25}H_{38}D_3NO_5S$ with 4.4% H_2O)