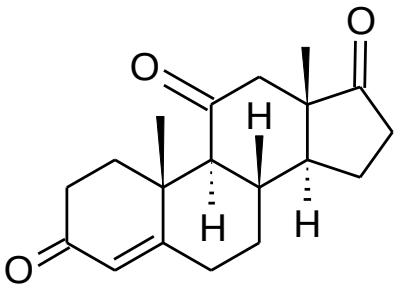
Our Formula. Your Success.

Compound Data Sheet

Structure:



Name	Androst-4-ene-3,11,17-trione
Synonym(s)	(+)-Adrenosterone, Δ4-Androstene-3,11,17-trione
Epichem Code #	EPL-DV6 Batch 2
CAS #	382-45-6
Molecular Formula	$C_{19}H_{24}O_3$
Molecular Weight	300.40 g/mol
Purity	99.6% at 242nm by HPLC (assuming all components detected with the same response factor). No impurities detected by ^1H NMR analysis. LC/MS: [M+H]+ = 301.2 IR ν_{max} cm^{-1} 1738(m), 1703(m), 1662(s)
Appearance	White solid
Melting point	218.9-224.1°C
Date of Manufacture	3 April 2019
Storage Requirements	Avoid exposure to heat, light and moisture.
Special Precautions	**This compound is for laboratory use only. Its toxicological properties may not have been fully established. It should be handled only by suitably qualified personnel.**

Document prepared by:

John Moursounidis
Head of Reference Standards
31 July 2019

Checked by:

Boon Tan
Quality Manager
31 July 2019

Epichem Pty Ltd, Suite 5, 3 Brodie-Hall Drive, Bentley WA 6102, Australia
Tel + 61 (0)8 6167 5200 Fax + 61 (0)8 6167 5201 www.epichem.com.au ABN 80 106 769 902

I. Identity

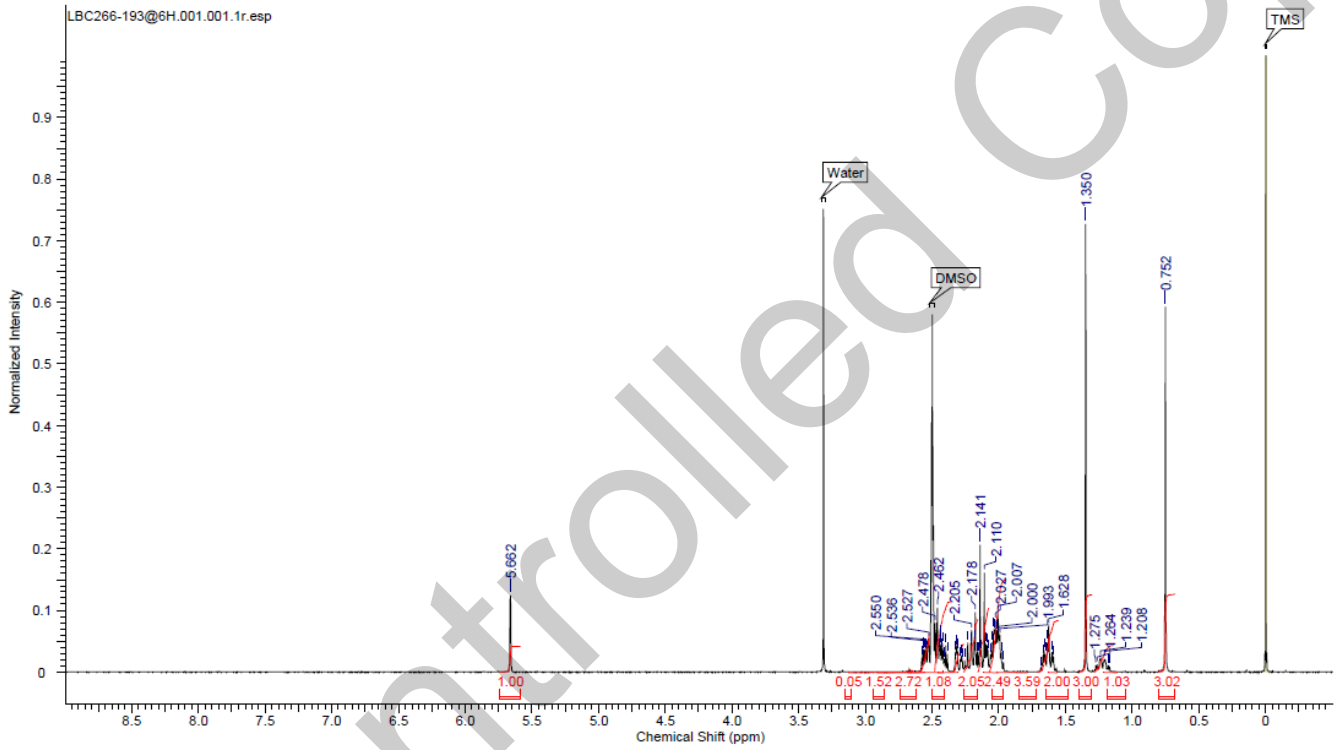
The identity of this product was established using the following analyses:

Ia. [1]HNMR Spectrum

Conditions: 400 MHz, DMSO-d6

[1]HNMR spectrum consistent with chemical structure.

Acquisition Time (sec)	3.7547	*Comment*	LBC266-193@6H 1H DMSO (E:\dataexternal\epichem) cygoh 8				
Date	29 May 2019 17:36:00			*Date Stamp*	29 May 2019 17:36:00		
File Name	\\naphthalene\company\NMR files\LBC266-193@6H\1\pdata\1\1r					*Frequency (MHz)*	400.13
Nucleus	1H	*Number of Transients*	8	*Origin*	spect	*Original Points Count*	24038
Owner	nmr	*Points Count*	32768	*Pulse Sequence*	zg	*Receiver Gain*	181.00
SW(cyclical) (Hz)	6402.05	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)*	2797.5447	*Spectrum Type*	STANDARD
Sweep Width (Hz)	6401.85	*Temperature (degree C)*	24.996				

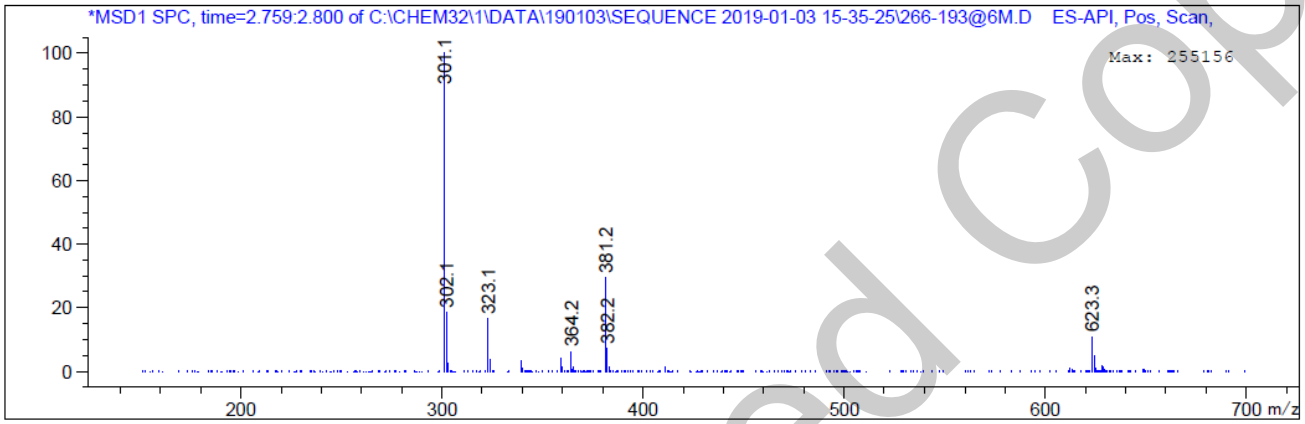


Epichem Pty Ltd, Suite 5, 3 Brodie-Hall Drive, Bentley WA 6102, Australia
Tel + 61 (0)8 6167 5200 Fax + 61 (0)8 6167 5201 www.epichem.com.au ABN 80 106 769 902

Ib. Mass Spectrum

The mass spectrum of this material was analysed by Liquid Chromatography Mass Spectroscopy (LCMS) using in-house EM005.WI08.

Retention Time (MS)	MS Area	Mol. Weight or Ion
2.776	2883845	623.30 I
		381.20 I
		323.10 I
		302.15 I
		301.10 I



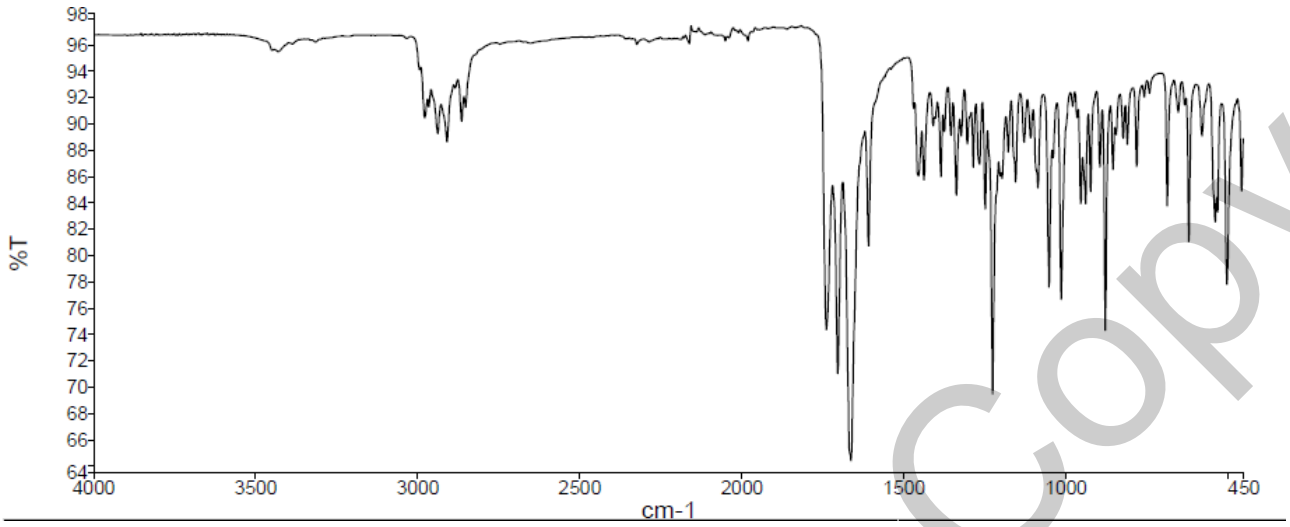
Theoretical value: 301.2 $[M+H]^+$.

The signal of the Mass Spectrum is consistent with the theoretical value and its interpretation is consistent with the structural formula.

Epichem Pty Ltd, Suite 5, 3 Brodie-Hall Drive, Bentley WA 6102, Australia
Tel + 61 (0)8 6167 5200 Fax + 61 (0)8 6167 5201 www.epichem.com.au ABN 80 106 769 902

Ic. IR Spectrum

The infra-red spectrum of this material was analysed by Fourier-Transform Infrared Spectroscopy (FTIR) using in-house EM005.WI09.



The interpretation of the signals of the Fourier-Transform Infrared Spectrum is consistent with the structural formula.

Epichem Pty Ltd, Suite 5, 3 Brodie-Hall Drive, Bentley WA 6102, Australia

Tel + 61 (0)8 6167 5200 Fax + 61 (0)8 6167 5201 www.epichem.com.au ABN 80 106 769 902

II. Purity

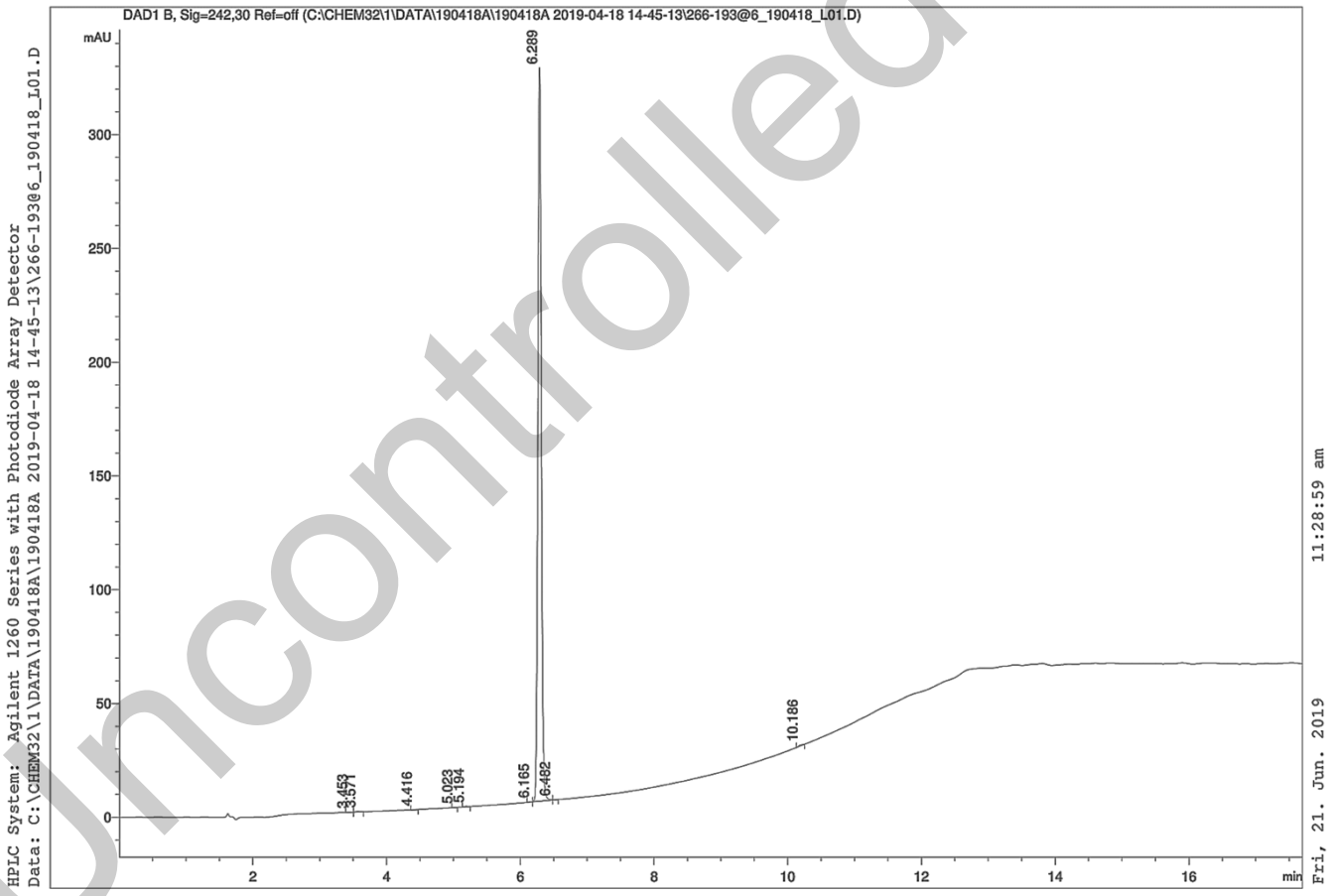
The purity of this material was analysed by high performance liquid chromatography (HPLC) using in-house EM005.WI07.

HPLC Conditions:

<table>
<tr><td>Column</td><td colspan="4">Conditions</td><td>Detector</td><td>Injector</td></tr>
<tr><td rowspan="8">Agilent Zorbax SB-C18

4.6 x 250mm

5.0 micron</td><td colspan="4">25ºC</td><td rowspan="8">DAD
242nm</td><td rowspan="8">Auto
1.0 µL
1.0 mg/mL 100% acetonitrile</td></tr>
<tr><td>Time (min)</td><td>% Line A (Water + 0.1% (v/v) TFA)</td><td>% Line B (Acetonitrile + 0.1% (v/v) TFA)</td><td>Flow rate (mL/min)</td></tr>
<tr><td>0.00</td><td>70</td><td>30</td><td>1.5</td></tr>
<tr><td>5.30</td><td>40</td><td>60</td><td>1.5</td></tr>
<tr><td>10.30</td><td>5</td><td>95</td><td>1.5</td></tr>
<tr><td>15.90</td><td>5</td><td>95</td><td>1.5</td></tr>
<tr><td>16.50</td><td>70</td><td>30</td><td>1.5</td></tr>
<tr><td>22.20</td><td>70</td><td>30</td><td>1.5</td></tr>
</table>



Epichem Pty Ltd, Suite 5, 3 Brodie-Hall Drive, Bentley WA 6102, Australia
Tel + 61 (0)8 6167 5200 Fax + 61 (0)8 6167 5201 www.epichem.com.au ABN 80 106 769 902

Area Percent Report – Sorted by Signal

Peak Number	Retention Time (rounded)	Area	Area % (rounded)
1	3.45	0.46	0.04
2	3.57	1.06	0.09
3	4.42	0.16	0.01
4	5.02	0.11	0.01
5	5.19	0.57	0.05
6	6.16	0.29	0.03
7	6.29	1135.52	99.59
8	6.48	0.42	0.04
9	10.19	1.62	0.14
Totals			100 (rounded)

For the calculation the system peaks were ignored. The content of the analyte was determined as a ratio of the peak area of the analyte and the cumulative areas of the purities, added up to 100%.

Results:

Average 99.6% (average duplicate analyses)

Epichem Pty Ltd, Suite 5, 3 Brodie-Hall Drive, Bentley WA 6102, Australia

Tel + 61 (0)8 6167 5200 Fax + 61 (0)8 6167 5201 www.epichem.com.au ABN 80 106 769 902