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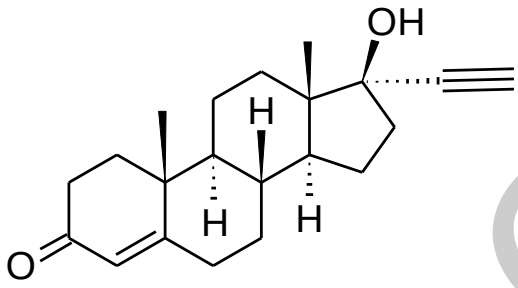
Compound Data Sheet

Structure:



Name	Ethisterone
Synonym(s)	17α-Ethynyl-17β-hydroxy-4-androsten-3-one; 17α-ethynyltestosterone
Epichem Code #	EPL-DV3 Batch 1
CAS #	434-03-7
Molecular Formula	$C_{21}H_{28}O_2$
Molecular Weight	312.46 g/mol
Purity	99.8% at 242nm by HPLC (assuming all components detected with the same response factor). No impurities detected by ^1H NMR analysis. LC/MS: [M+H]+ = 313.2 IR ν_{max} cm^{-1} 3401(m), 3259(m), 1658(s)
Appearance	White solid
Melting point	269.5-272.5°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:

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30 July 2019

Checked by:

Boon Tan
Quality Manager
30 July 2019

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I. Identity

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

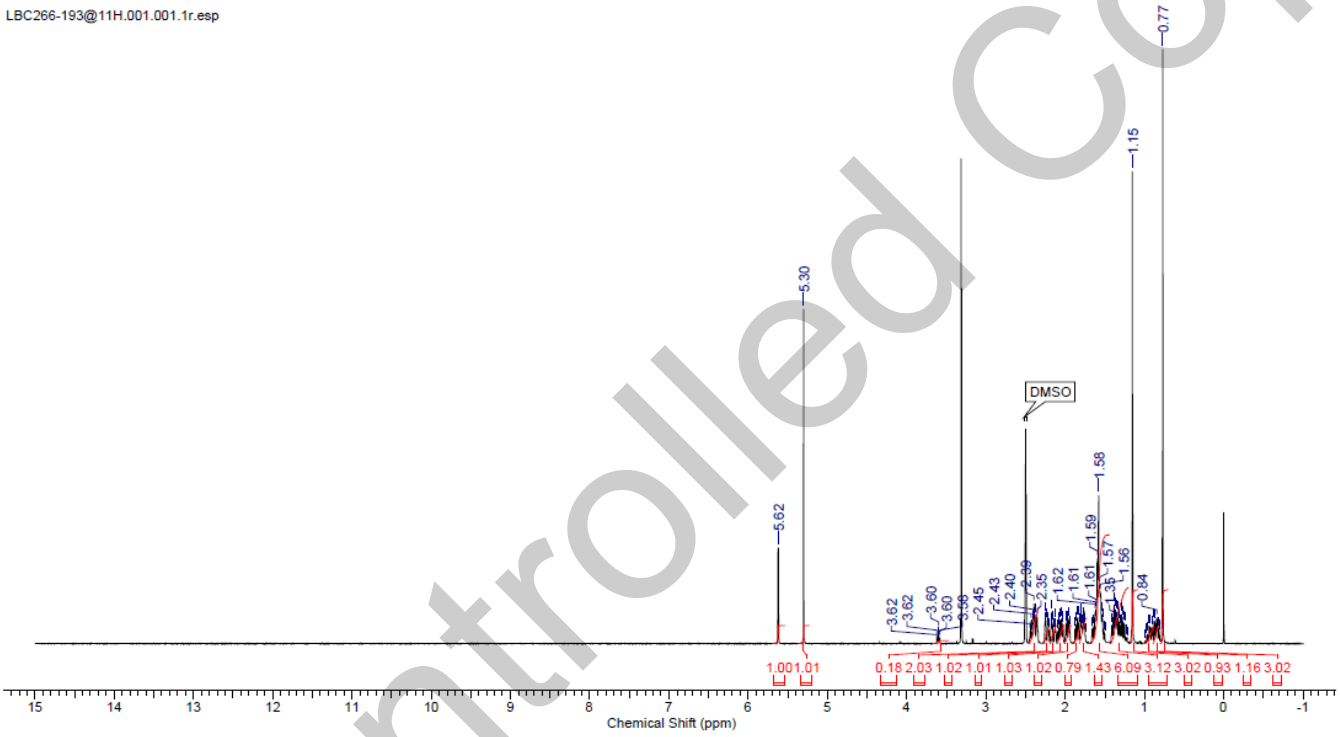
Ia. [1]HNMR Spectrum

Conditions: 400 MHz, DMSO-d6

[1]HNMR spectrum consistent with chemical structure.

Acquisition Time (sec)	3.7547	*Comment*	LBC266-193@11H 1H DMSO {E:\dataexternal\epichem} cygoh 2				
Date	12 Jun 2019 17:10:24			*Date Stamp*	12 Jun 2019 17:10:24		
File Name	\\naphthalene\company\NMR files\LBC266-193@11H\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*	144.00
SW(cyclical) (Hz)	6402.05	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)*	2797.6125	*Spectrum Type*	STANDARD
Sweep Width (Hz)	6401.85	*Temperature (degree C)*	24.996				

LBC266-193@11H.001.001.1r.esp



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Ib. Mass Spectrum

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

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MS Signal: MSD1 TIC, MS File,  ES-API, Pos, Scan, Frag: 70
    Spectra averaged over upper half of peaks.
    Noise Cutoff: 1000 counts.
    Reportable Ion Abundance: > 10%.


Retention                    Mol. Weight
Time (MS)      MS Area       or Ion

   3.117       2108824        393.20 I
                              314.20 I
                              313.20 I
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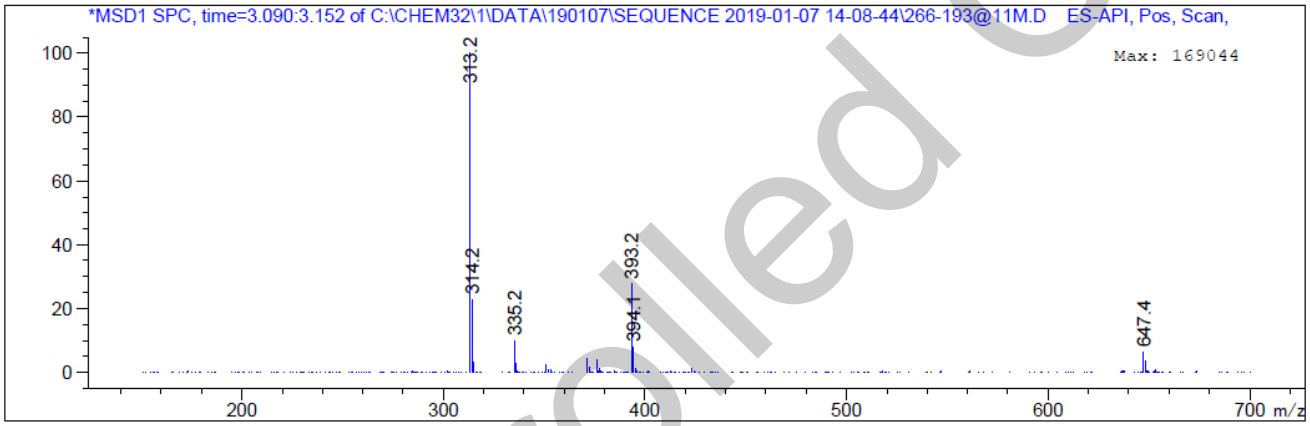

Theoretical value: 313.2 $[M+H]^+$.

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

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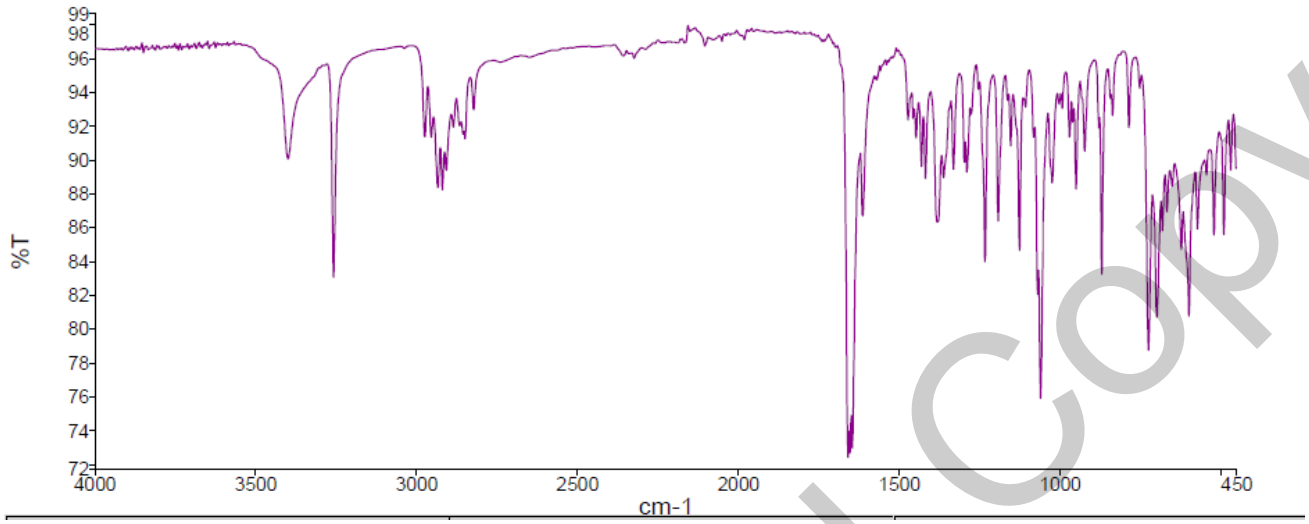
Ic. IR Spectrum

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.

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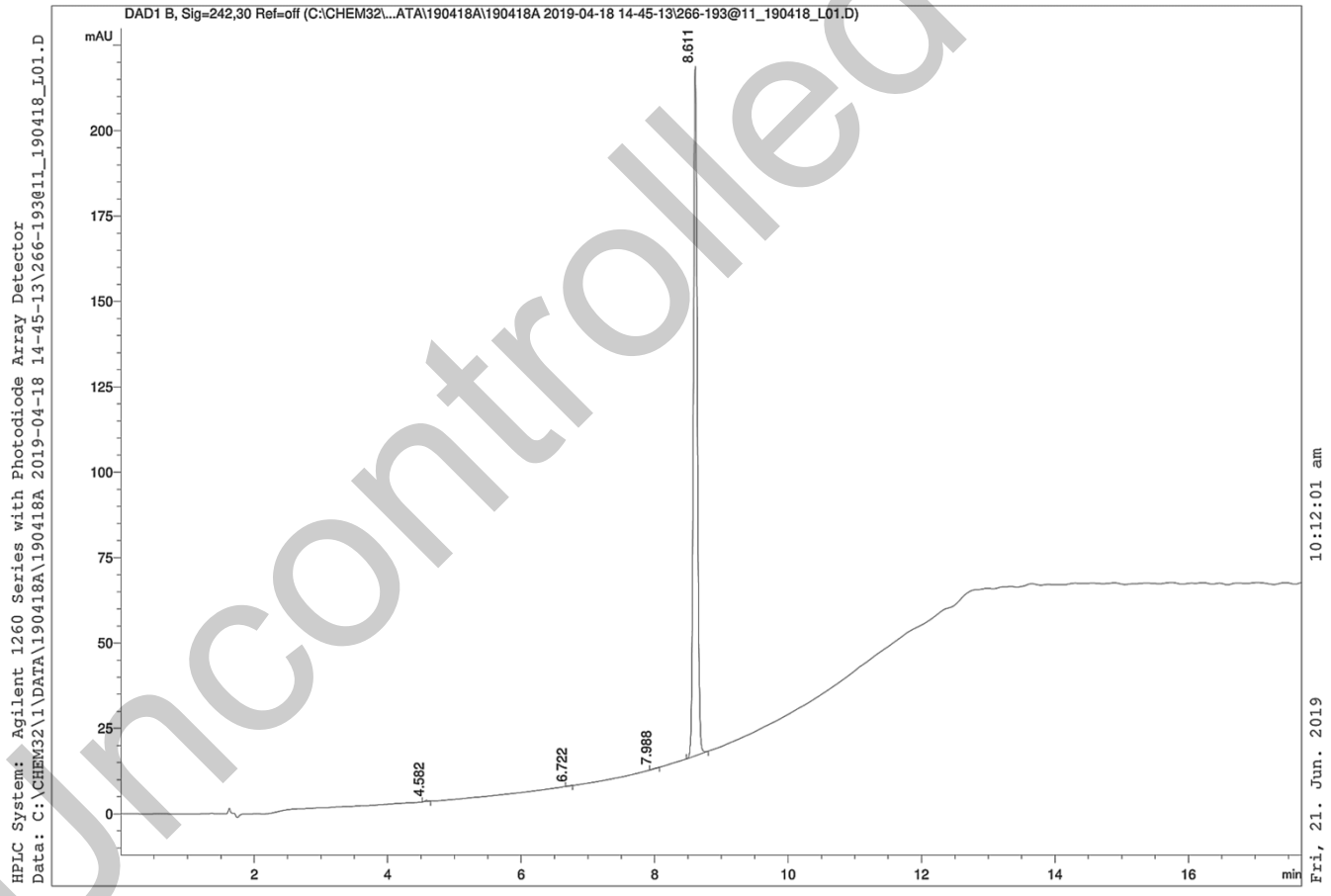
II. Purity

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

HPLC Conditions:

Column	Conditions				Detector	Injector
Agilent Zorbax SB-C18 4.6 x 250mm 5.0 micron	25ºC				DAD 242nm	Auto 1.0 µL 1.0 mg/mL 100% acetonitrile
	Time (min)	% Line A (Water + 0.1% (v/v) TFA)	% Line B (Acetonitrile + 0.1% (v/v) TFA)	Flow rate (mL/min)		
	0.00	70	30	1.5		
	5.30	40	60	1.5		
	10.30	5	95	1.5		
	15.90	5	95	1.5		
	16.50	70	30	1.5		
	22.20	70	30	1.5		



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Area Percent Report – Sorted by Signal

Peak Number	Retention Time (rounded)	Area	Area % (rounded)
1	4.58	1.12	0.14
2	6.72	0.18	0.02
3	7.99	0.51	0.06
4	8.61	812.32	99.78
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 98.0% (average duplicate analyses)

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