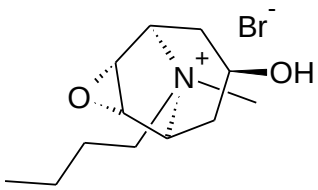
ISO 9001 CERTIFIED QUALITY MANAGEMENT

Our Formula. Your Success.

Reference Material Product Information Sheet

Epichem's Quality System conforms to ISO9001:2015 as certified by ECAAS Pty Ltd - Certification number 616061.



Name	(1α,2β,4β,5α,7β)-9-butyl-7-hydroxy-9-methyl-3-oxa-9-azoniatricyclo[3.3.1.$0^{2,4}$]nonane bromide (1:1)
Synonym(s)	Scopine Butyl Bromide
Epichem Item #	EPL-AA254 Batch 1
CAS #	2030294-83-6
Molecular Formula	$C_{12}H_{22}NO_2$. Br
Molecular Weight	292.22 g/mol
Appearance	White powder
Melting Point	183.8°C – 189.0°C (Decomposition)
Combustion Analysis	Required (%): C: 49.3, H: 7.6., N: 4.8. Found (%): C: 49.4, H: 7.6, N: 4.8.
Ion Chromatography	Required (%): Br: 27.3, Cl: 0.0, SO_4^{2-}: 0.0. Found (%) Br: 27.0, Cl: <0.01, SO_4^{2-} <0.01.
Purity	100.0 ± 0.4% by qNMR
Date of Manufacture	7 October 2019
Storage Requirements	Protect from 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.**
Intended Use	This compound is suitable for the identification of impurities and degradants in pharmaceutical materials. The purity assay is considered as relative contribution.
Date of Shipment	TBA
	This certificate is valid for one year from the date of shipment provided the substance is unopened and stored under the recommended conditions.
Retest Date	TBA (Proper Storage and Handling Required)

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

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

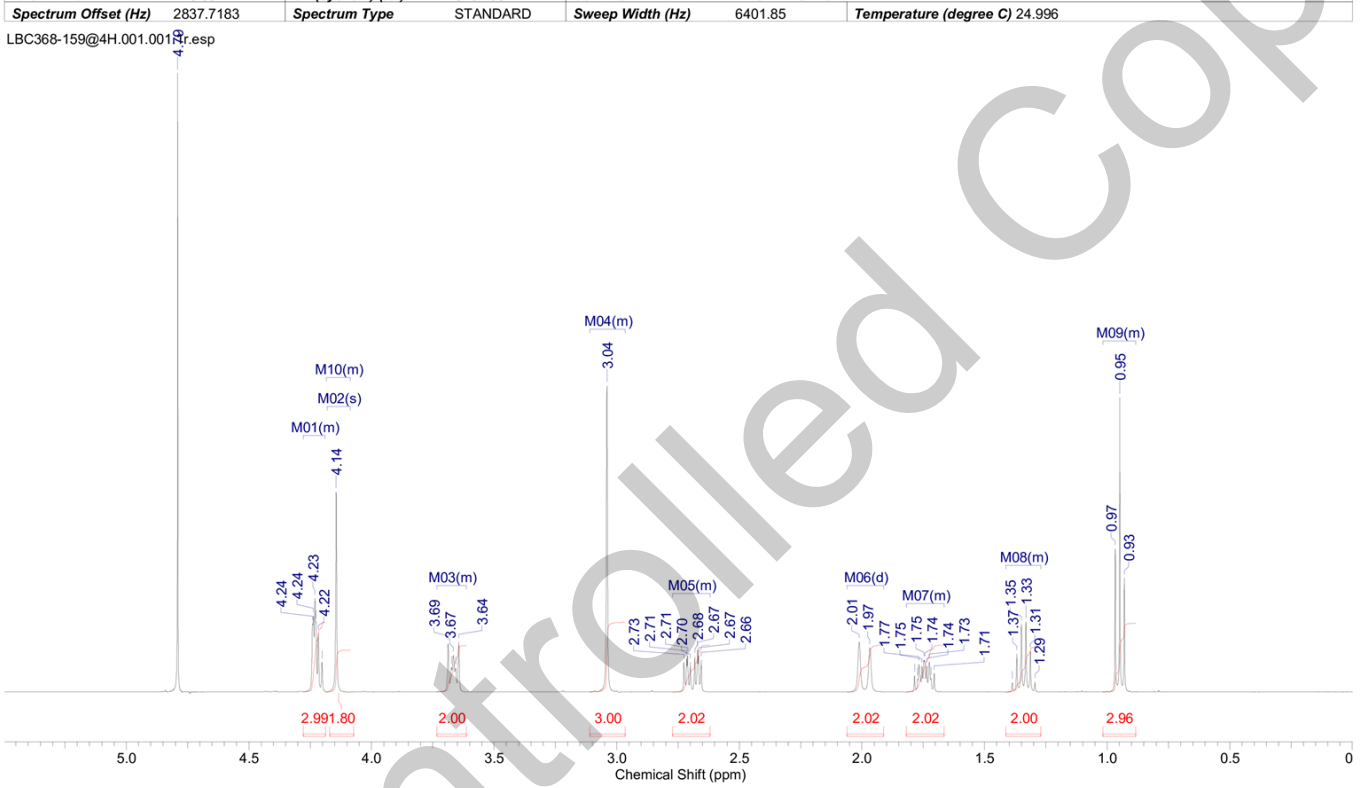
Ia. ^{1}HNMR Spectrum

Conditions: 400 MHz, D_2O

^{1}HNMR spectrum consistent with chemical structure.

Acquisition Time (sec)	3.7547	***Comment***	LBC368-159@4H 1H D2O {E:\dataexternal\epichem} cygoh 10	***Date***	15 Oct 2019 17:23:12		
Date Stamp	15 Oct 2019 17:23:12			***File Name***	\\naphthalene\company\NMR files\LBC368-159@4H\1\pdata\1\1r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	spect
Original Points Count	24038	***Owner***	nmr	***Points Count***	32768	***Pulse Sequence***	zg
Receiver Gain	128.00	***SW(cyclical) (Hz)***	6402.05	***Solvent***	DEUTERIUM OXIDE		
Spectrum Offset (Hz)	2837.7183	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	6401.85	***Temperature (degree C)***	24.996

LBC368-159@4H.001.001r.esp



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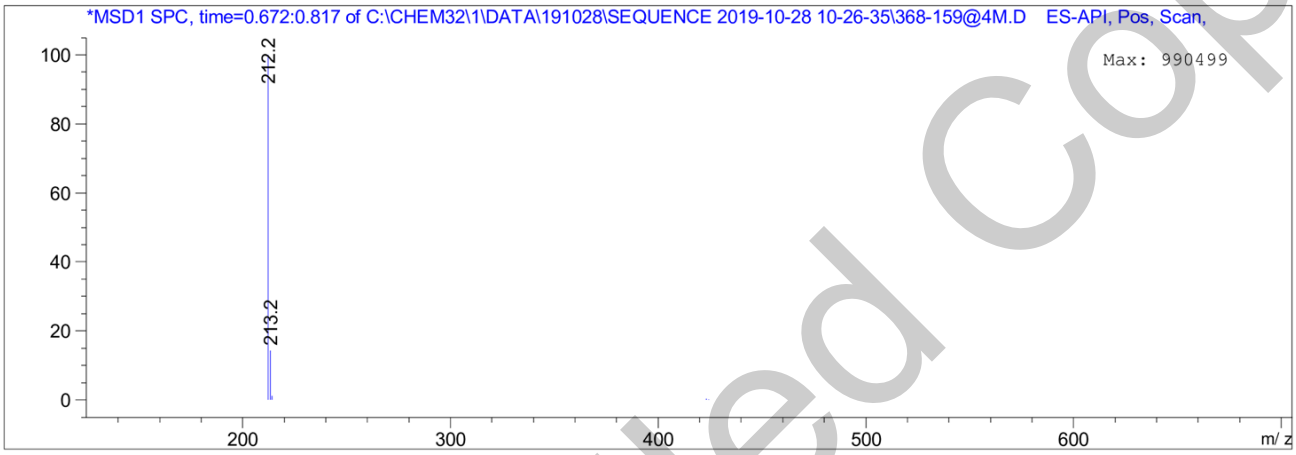
Ib. Mass Spectrum

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

Method: ACN/water gradient (+0.1% formic acid)

Zorbax SB-C8, 4.6 x 30 mm, 3.5 micron

Retention Time (MS)	MS Area	Mol. Weight or Ion
0.710	14238736	213.20 I
		212.20 I



Theoretical value: 212.2 $[M\text{-}Br]^+$

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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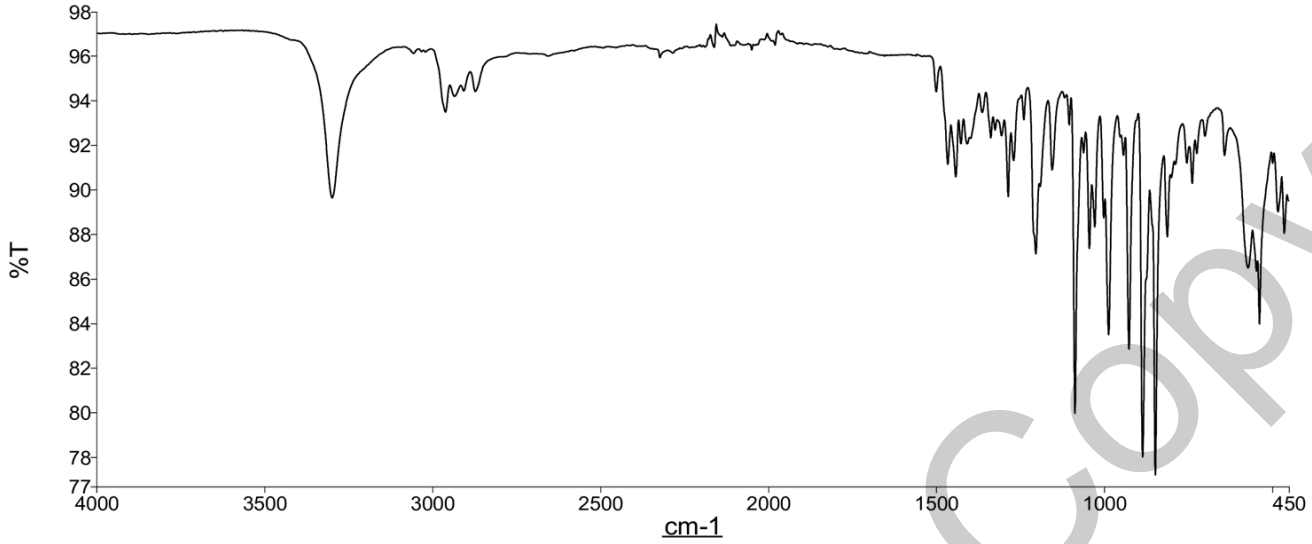
Ic. IR Spectrum

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



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

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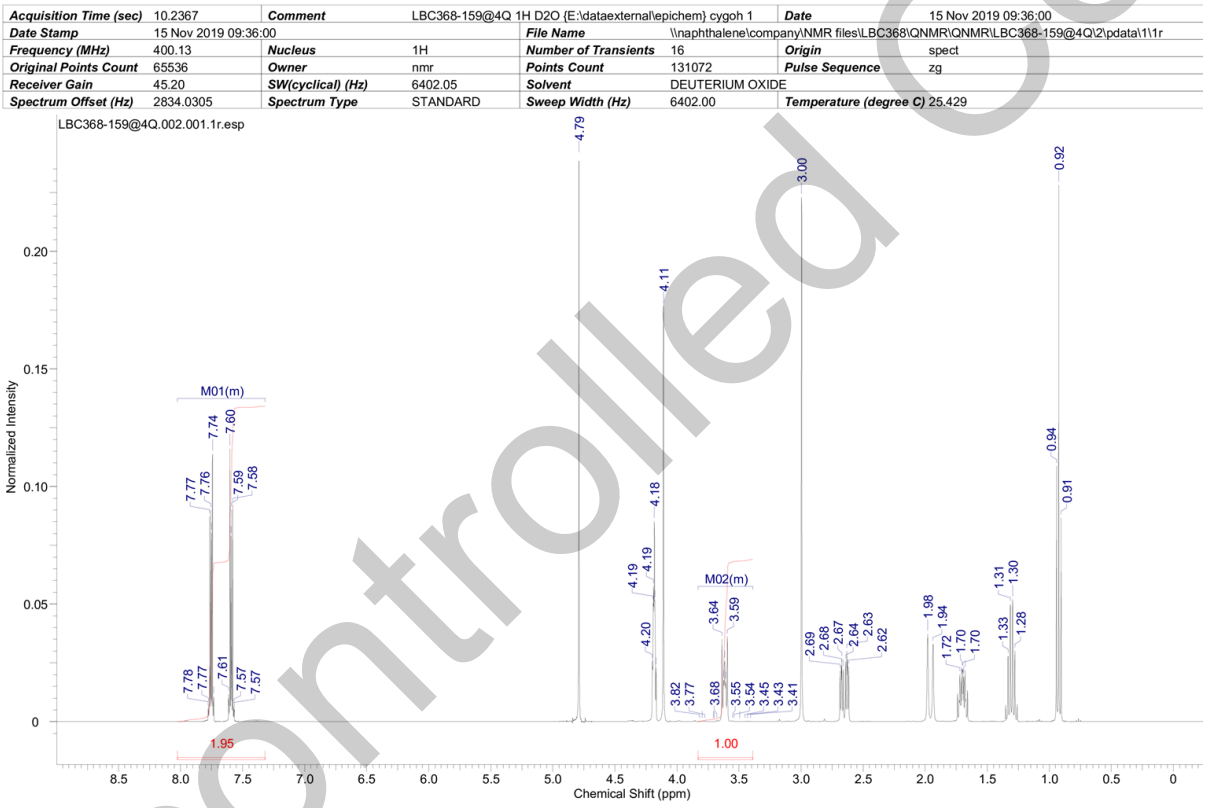
II. Purity

The purity of this material was analysed by Quantitative Hnmr (Q^{1}Hnmr).

Q^{1}Hnmr Conditions:

Instrument:	Bruker AVANCE III 400MHz NanoBay Spectrometer		
Operating Frequency:	400.13MHz (^{1}H)		
Frequency Reference:	Solvent: D_2O; δ 4.7ppm		
Pulse Angle:	90^o		
Acquisition Time:	10.2s	**Data Points:**	64k
Relaxation Delay:	60s	**Transients:**	16
Solvent:	D_2O		
Internal Standard:	Potassium phthalate monobasic 99.99±0.17% (Trace-CERT, Sigma-Aldrich)		



Purity Formula:

$$P\ [\%] = \frac{n_{IC} \cdot Int_t \cdot MW_t \cdot m_{IC}}{n_t \cdot Int_{IC} \cdot MW_{IC} \cdot m_s} \cdot P_{IC}$$

Where: **P** = Purity (%)
MW = Molecular Weight (g/mol)
IC = Internal Calibrant
s = sample
t = target analyte
Int = Integral for a given Hnmr signal
n = number of protons for a given Hnmr signal
m = mass (mg)
mol = mole

Result: Analyte purity **100.0 +/- 0.4%**
(result of triplicate runs)

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III. Water Content

Method: Karl-Fischer titration using in-house EM005.WI04.

Results:

Average 0.1%

IV. Residual Solvents

Method: ^{1}HNMR

Result:

No significant impurities detected by ^{1}H NMR analysis.

V. Final Result

qNMR Purity	100.0 ± 0.4%
Water content	0.1%
Residual solvents	<0.1%
Purity	100.0 ±0.4%

This purity is assessed to be 100.0%.

Product Reviewed By:

James Rixson, PhD
Head of Production

Product Released By:

Carol Worth
Quality Manager

Release Date: 18 May 2022

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