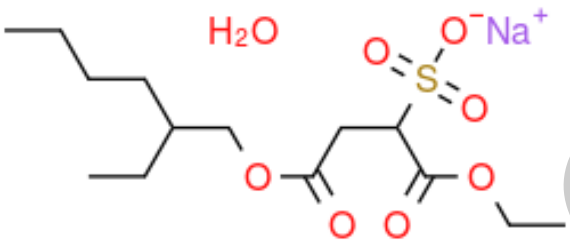
Our Formula. Your Success.

Reference Material Product Information Sheet

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



Name	sodium 1-ethoxy-4-((2-ethylhexyl)oxy)-1,4-dioxobutane-2-sulfonate monohydrate
BP/EP Name	Not Listed.
USP Name	Not Listed.
Synonym(s)	sodium 1-ethoxy-4-((2-ethylhexyl)oxy)-1,4-dioxobutane-2-sulfonate (monohydrate)
Epichem Item #	EPL-AA236 Batch 1
CAS #	2575516-80-0
Molecular Formula	$C_{14}H_{25}O_7S.Na.H_2O$
Molecular Weight	378.42 g/mol
Appearance	White powder
Melting Point	75.8°C – 82.2°C (decomposition)
Combustion Analysis	Required (%): C: 44.4, H: 7.2, N: 0.0. Found (%): C: 44.2, H: 7.2, N: 0.2.
ICP-MS	Theoretical (%): Na: 6.1, S: 8.5. Found (%) Na: 7.8, 6.9, S: 11.2, 9.1.
Purity	98.4%
Date of Manufacture	16 July 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)

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I. Identity

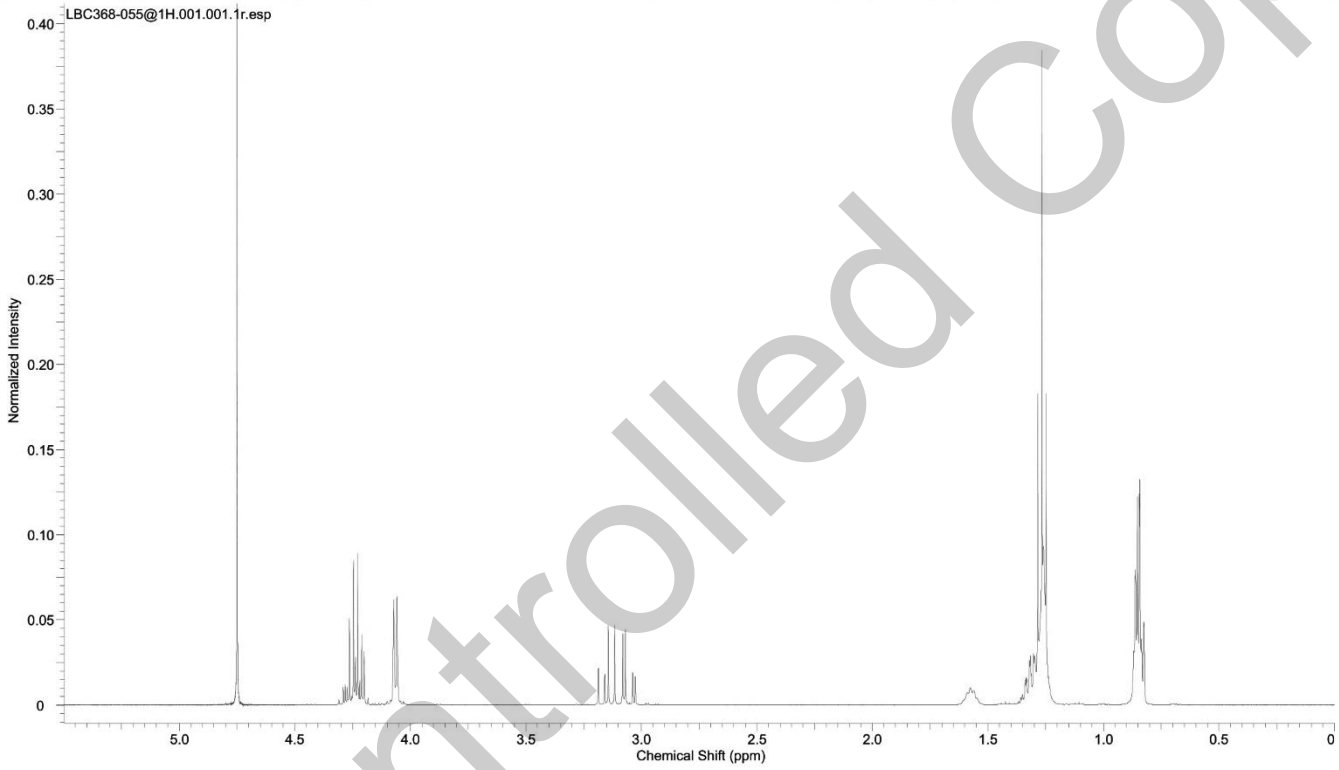
The identity of this product was established using the following analyses:

Ia. [1]HNMR Spectrum

Conditions: 400 MHz, D_2O

[1]HNMR spectrum consistent with chemical structure.

Acquisition Time (sec)	3.7547	***Comment***	LBC368-055@1H 1H D2O {E:\dataexternal\epichem} cygoh 23	***Date***	25 Jun 2019 17:38:08		
Date Stamp	25 Jun 2019 17:38:08			***File Name***	\\naphthalene\company\NMR files\LBC368-055@1H\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	114.00	***SW(cyclical) (Hz)***	6402.05	***Solvent***	DEUTERIUM OXIDE		
Spectrum Offset (Hz)	2819.3687	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	6401.85	***Temperature (degree C)***	24.996



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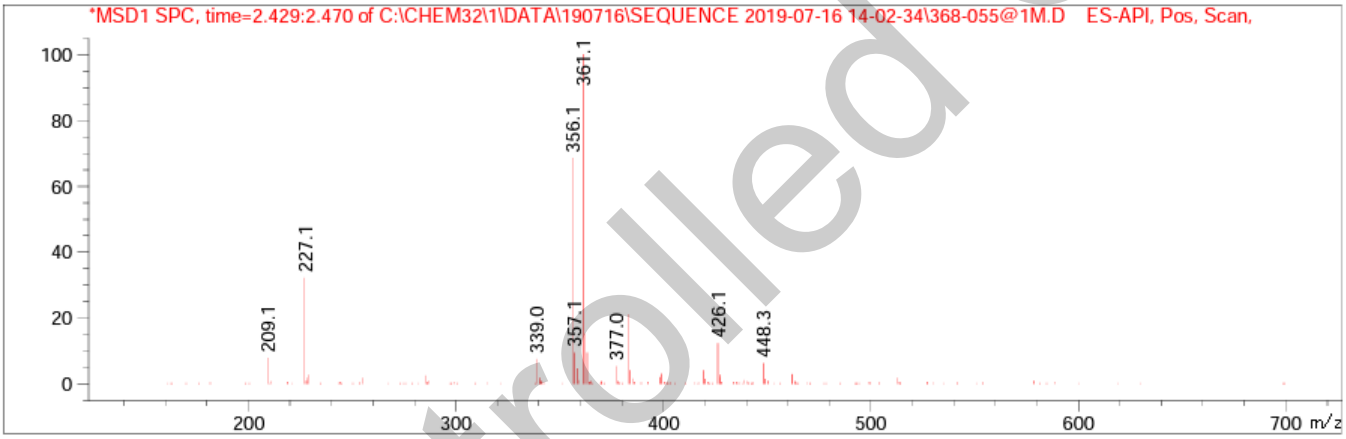
Ib. Mass Spectrum

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
2.310	49007	646.50 I
		645.10 I
2.449	883100	426.15 I
		383.15 I
		362.15 I
		361.15 I
		356.10 I
		227.05 I



Theoretical values: 361.1 $[M+Na]^+$.

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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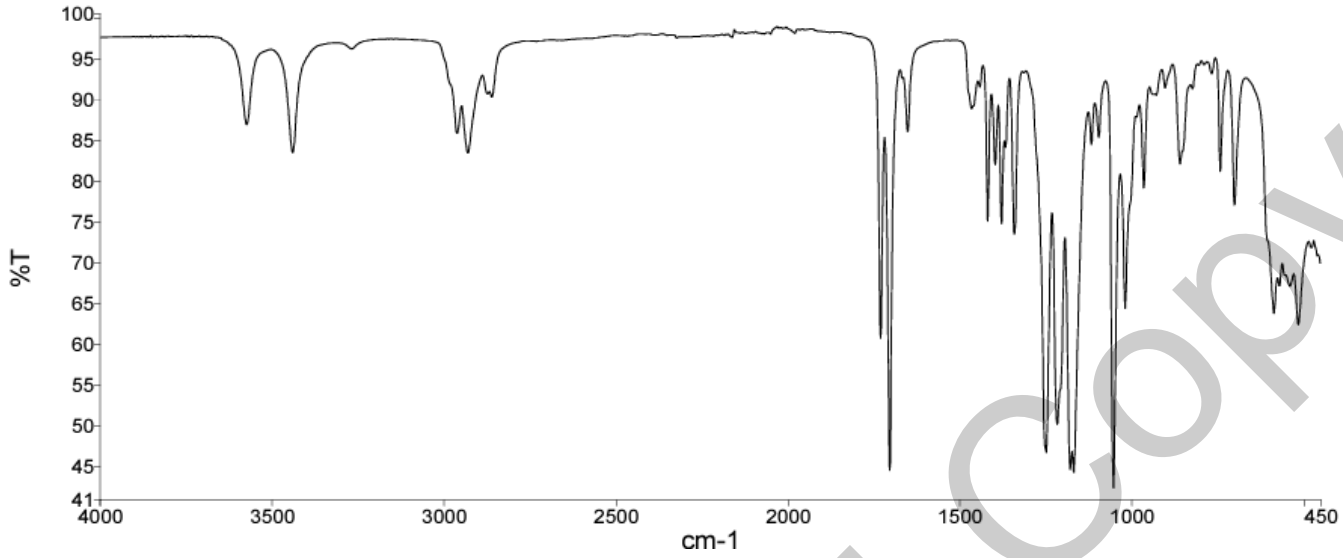
Ic. IR Spectrum

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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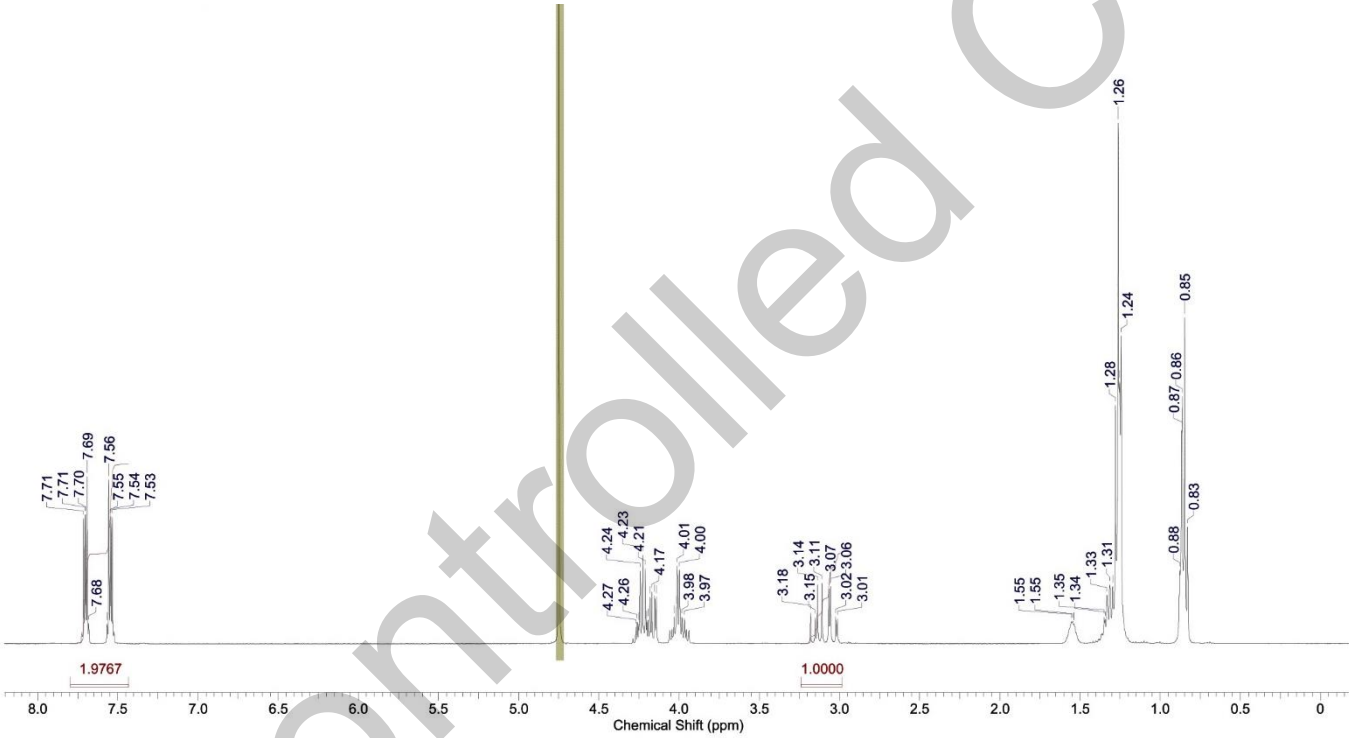
II. Purity

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

Q^{1}Hnmr Conditions:

Instrument:	Bruker AAVANCE III 400 MHz NanoBay		
Operating Frequency:	400.13MHz (^{1}H)		
Frequency Reference:	Solvent: D_2O; δ 4.75ppm		
Pulse Angle:	90°		
Acquisition Time:	10.0s	**Data Points:**	131k
Relaxation Delay:	60s	**Transients:**	16
Solvent:	D_2O		
Internal Standard:	Potassium phthalate monobasic 99.99% (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 98.4 +/- 0.8%

EPL-AA236 Batch 1

III. Water Content

Method: Karl-Fischer titration using in-house EM005.WI04.
Results:
Average 4.9%

IV. Residual Solvents

Method: ^{1}HNMR
Result:
No significant impurities detected by ^{1}H NMR analysis.

VI. Final Result

Q^{1}Hnmr Purity	98.4%
Water content	4.9%
Residual solvents	<0.1%
Purity	98.4%

This purity is assessed to be 98.4%.

Product Reviewed By:

Jacob Heppell, PhD
Chemist

Product Released By:

Carol Worth, PhD
Quality Manager

Release Date: 12 June 2023

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