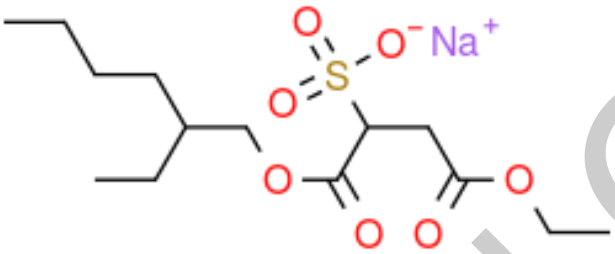
Our Formula. Your Success.

Reference Material Product Information Sheet

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



Name	sodium 4-ethoxy-1-((2-ethylhexyl)oxy)-1,4-dioxobutane-2-sulfonate
BP/EP Name	Not Listed.
USP Name	Docusate Sodium Related Compound D
Synonym(s)	Not Available.
Epichem Item #	EPL-AA219 Batch 1
CAS #	2575516-73-1
Molecular Formula	$C_{14}H_{25}O_7S.Na$
Molecular Weight	360.40 g/mol
Appearance	Beige solid foam
Combustion Analysis	Required (%): C: 46.7, H: 7.0. Found (%): C: 45.1, H: 7.1.
ICP-AES	Theoretical (%): Na: 6.4, S: 8.9. Found (%) Na: 6.7, S: 8.9.
Purity	91.8%
Date of Manufacture	10 May 2017
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

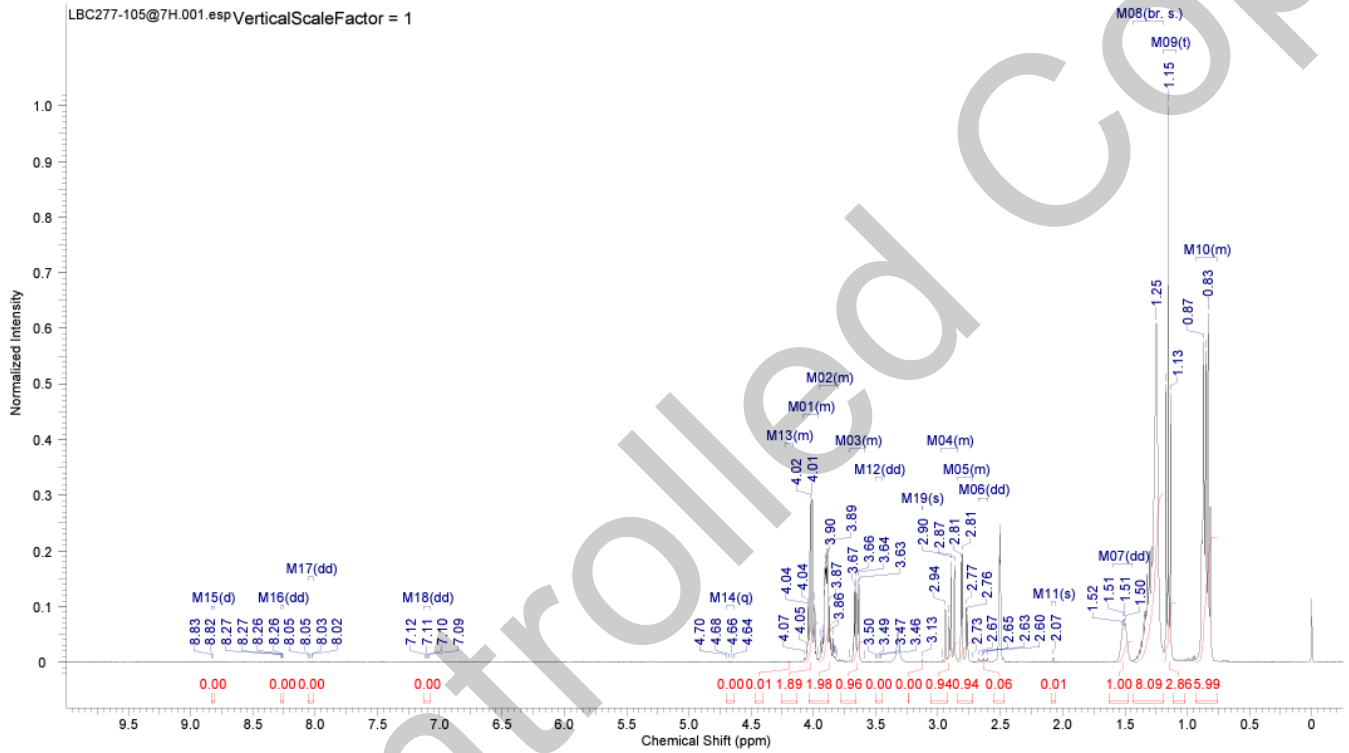
The identity of this product was established using the following analyses:

Ia. [1]HNMR Spectrum

Conditions: 400 MHz, D_2O

[1]HNMR spectrum consistent with chemical structure.

Acquisition Time (sec)	3.7547	*Comment*	LBC277-105@7H 1H DMSO {E:\dataexternal\epichem} cygoh 15				
Date	10 May 2017 17:42:24			*Date Stamp*	10 May 2017 17:42:24		
File Name	\\NAPHTHALENE\Company\NMR files\LBC277-105@7H\1\fid					*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*	45.20
SW(cyclical) (Hz)	6402.05	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)*	2798.4006	*Spectrum Type*	STANDARD
Sweep Width (Hz)	6401.85	*Temperature (degree C)*	26.945				



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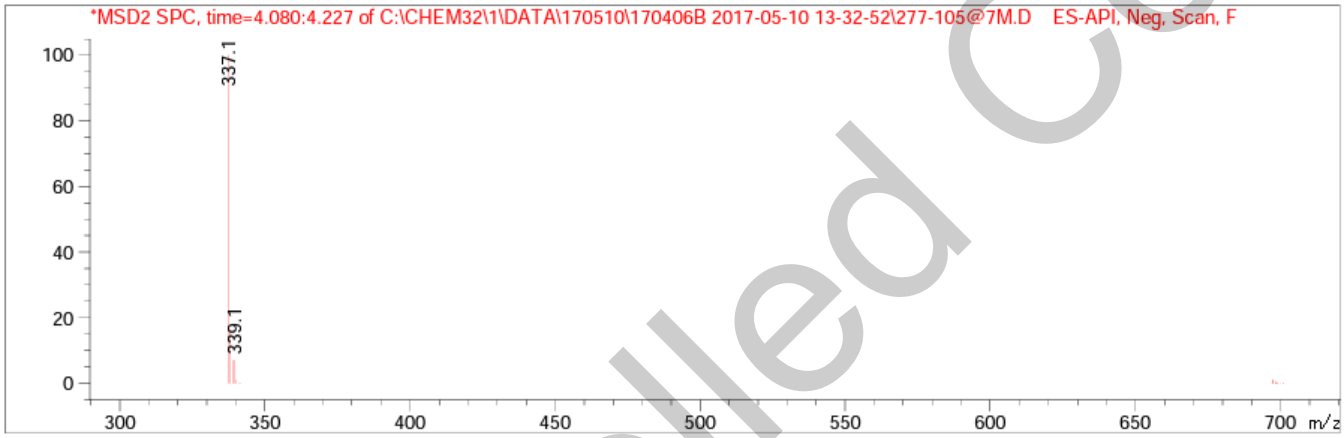
Ib. Mass Spectrum

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

Method: 5% to 100% ACN in water gradient (+0.1% formic acid)

Zorbax Eclipse XDB-C8, 3.0 x 100 mm, 3.5 micron

Retention Time (MS)	MS Area	Mol. Weight or Ion
3.565	145971	310.10 I
		309.15 I
4.114	2712831	338.10 I
		337.15 I



Theoretical values: 337.1 $[M-H]^-$.

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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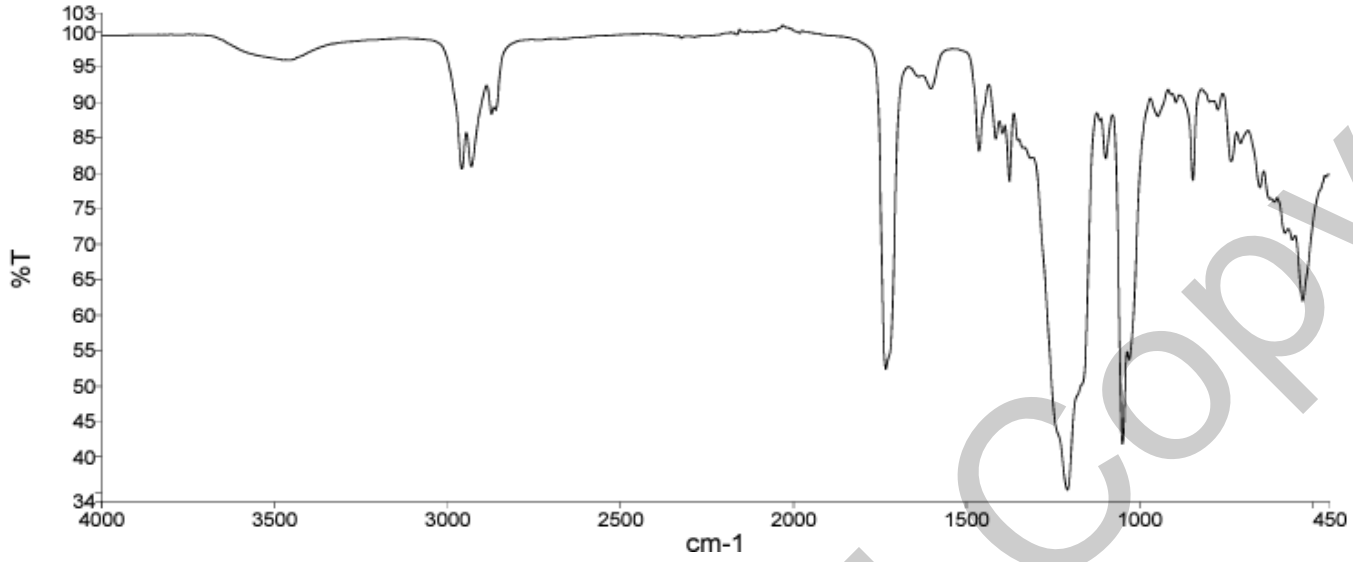
Ic. IR Spectrum

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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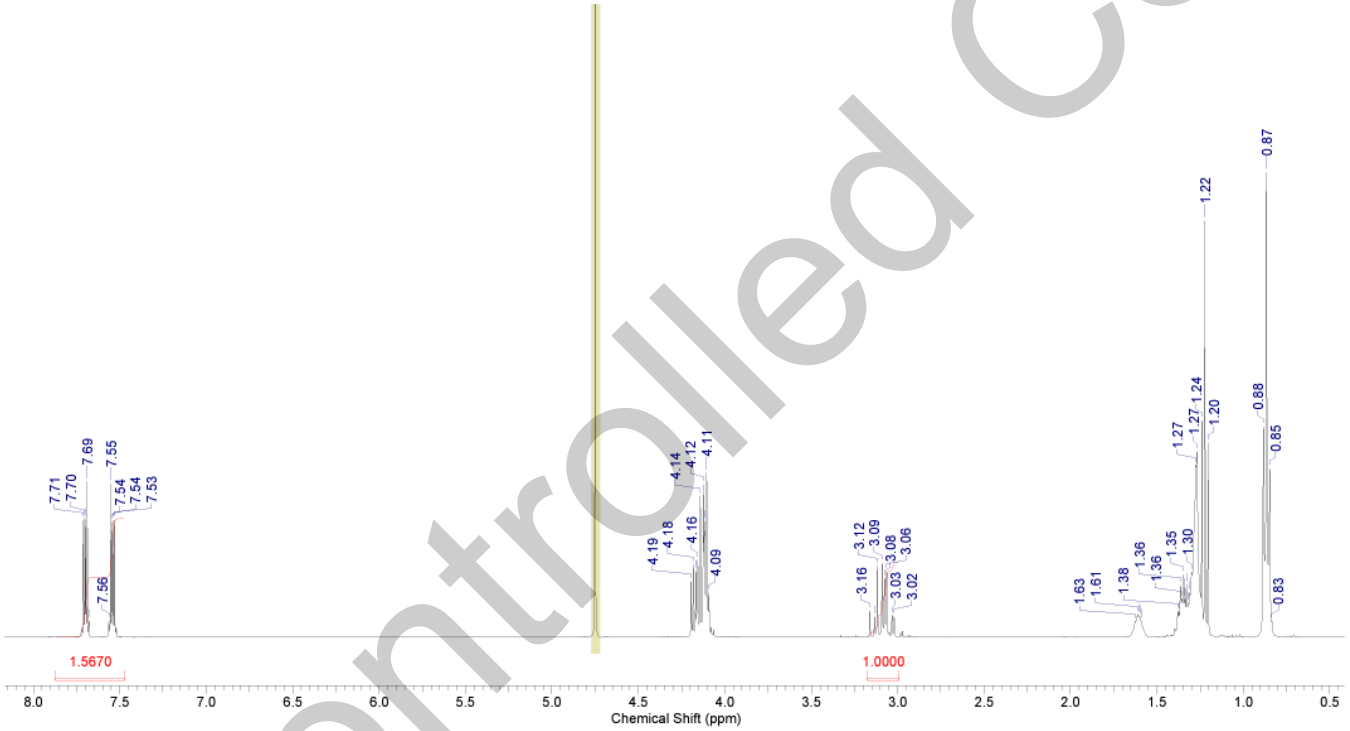
II. Purity

The purity of this material was analysed by 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 91.8 +/- 0.5%

EPL-AA219 Batch 1

III. Water Content

Method: Karl-Fischer titration using in-house EM005.WI04.
Results:
Average 2.6%

IV. Residual Solvents

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

VI. Final Result

Q^{1}Hnmr Purity	91.8%
Water content	2.6%
Residual solvents	<0.1%
Purity	91.8%

This purity is assessed to be 91.8%.

Product Reviewed By:

James Rixson, PhD
Head of Production

Product Released By:

Carol Worth, PhD
Quality Manager

Release Date: 9 June 2023

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