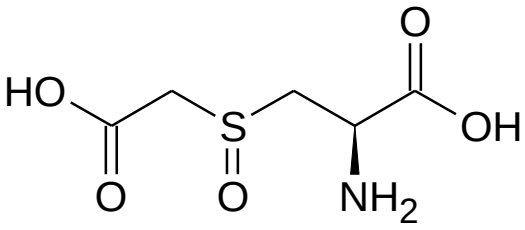
Our Formula. Your Success.

Reference Material Product Information Sheet

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



Name	*S*-carboxymethyl-*L*-cysteine sulfoxide
Synonym(s)	(2*R*)-2-amino-3-((carboxymethyl)sulfinyl)propanoic acid
Epichem Item #	EPL-AA79 Batch 2
CAS #	5439-87-2
Molecular Formula	$C_5H_9NO_5S$
Molecular Weight	195.20 g/mol
Appearance	White powder
Melting Point	156.3-161.7°C (decomposition).
Combustion Analysis	Required (%): C:30.8; H:4.6; N:7.2. Found (%): C: 30.6; H: 4.6; N: 7.0.
Purity	99.2%
Date of Manufacture	5 October 2020
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 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

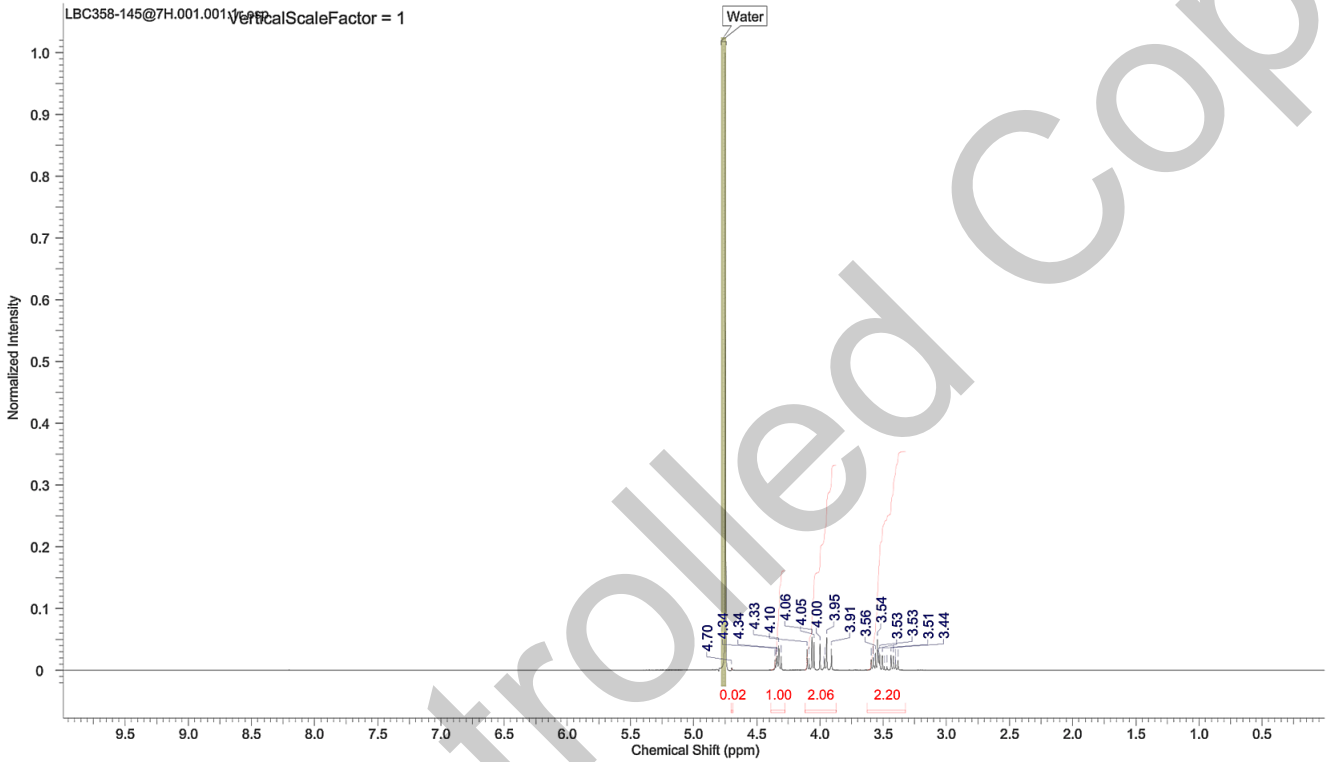
The identity of this product was established using the following analyses:

Ia. ^{1}HNMR Spectrum

Conditions: 400 MHz, D_2O

^{1}HNMR spectrum consistent with chemical structure.

Acquisition Time (sec)	3.7547	*Comment*	LBC358-145@7H 1H D2O {E:\dataexternal\epichem} cygoh 6			*Date*	16 Sep 2020 17:25:20
Date Stamp	16 Sep 2020 17:25:20			*File Name*	\\naphthalene\company\NMR files\LBC358-145@7H\1\pdata\1\1r		
Frequency (MHz)	400.13	*Nucleus*	1H	*Number of Transients*	32	*Origin*	spect
Original Points Count	24038	*Owner*	nmr	*Points Count*	32768	*Pulse Sequence*	zg
Receiver Gain	203.00	*SW(cyclical) (Hz)*	6402.05	*Solvent*	DEUTERIUM OXIDE		
Spectrum Offset (Hz)	2818.9778	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	6401.85	*Temperature (degree C)*	24.996



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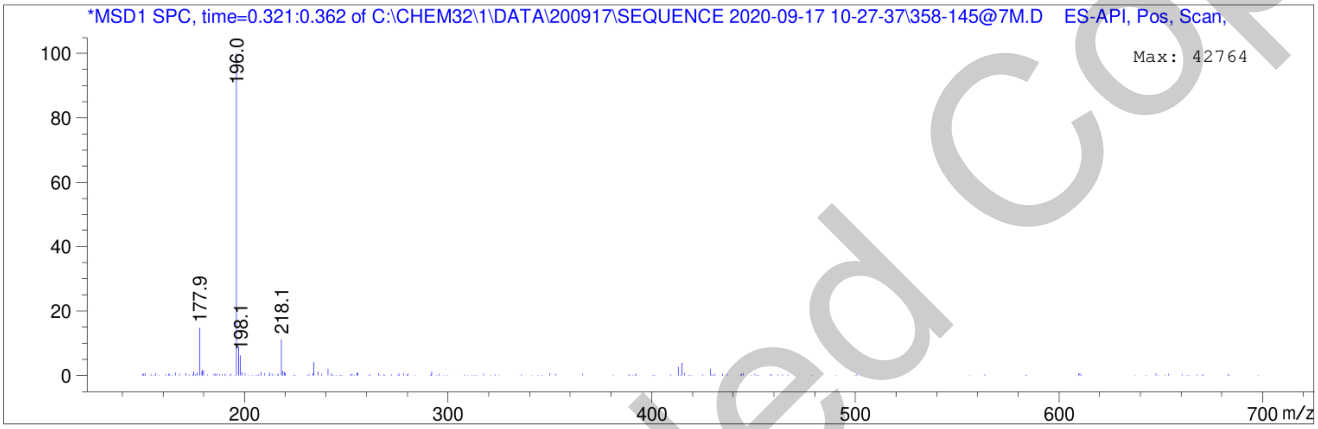
Ib. Mass Spectrum

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
0.330	364486	218.05 I
		196.00 I
		177.95 I



Theoretical value: 196.0 $[M+H]^+$.

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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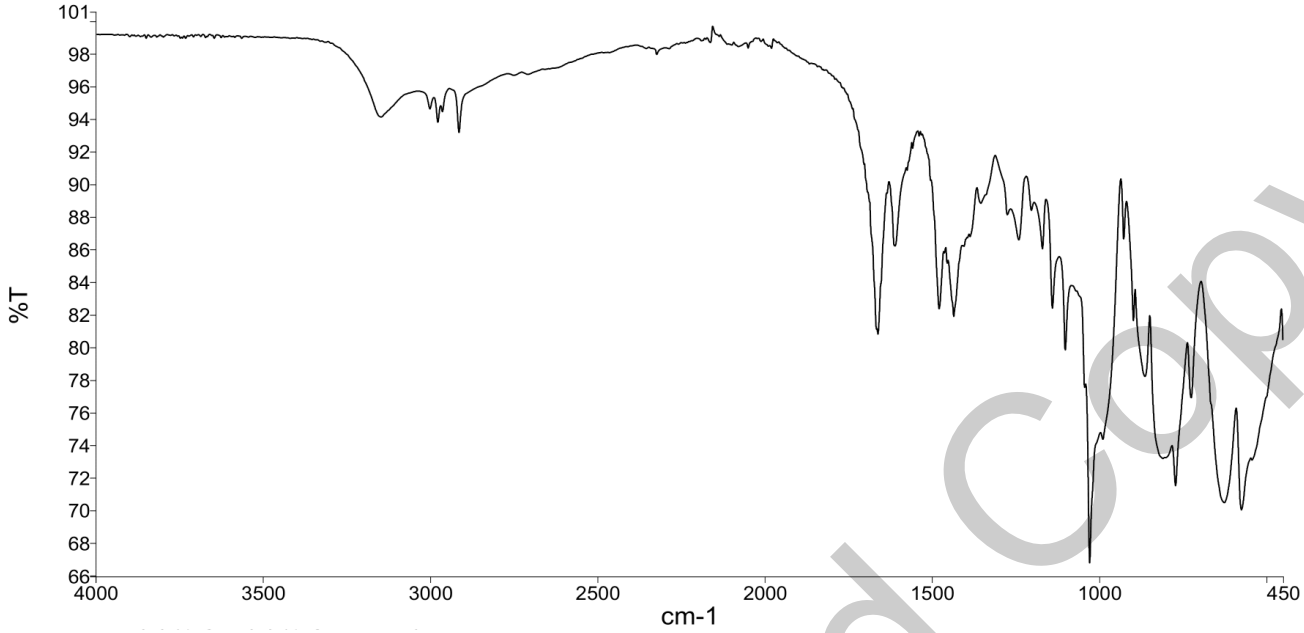
Ic. IR Spectrum

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 Poroshell 120 HILIC 4.6 x 100mm 2.7 micron	25ºC				DAD 220nm	Auto 1.0 µL 2.4 mg/mL in 100% water (NO MODIFIERS)
	Time (min)	% Line A (Water + 0.1% (v/v) TFA)	% Line B (Acetonitrile + 0.1% (v/v) TFA)	Flow rate (mL/min)		
	0.00	3	97	1.0		
	4.00	5	95	1.0		
	7.00	8	92	1.0		
	11.00	16	84	1.0		
	15.00	40	60	1.0		
	17.00	40	60	1.0		
	18.00	3	97	1.0		
	28.40	3	97	1.0		

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Area Percent Report – Sorted by Signal

Peak Number	Retention Time (rounded)	Area	Area % (rounded)
1	1.27	0.84	0.08
2	1.36	0.77	0.07
3	2.50	1.10	0.10
4	4.12	1061.92	99.68
5	8.34	0.67	0.06
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 99.7% (average of duplicate runs)

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III. Water Content

Method: Karl-Fischer titration using in-house EM005.WI04.
Results:
Average 0.4%

IV. Ash Content

Method: BP2020 Appendix XI J Method II
Result:
Contains 0.1% ash.

V. Residual Solvents

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

VI. Final Result

Chromatographic purity (HPLC)	99.7%
Water content	0.4%
Ash content	0.1%
Residual solvents	<0.1%
Purity	99.2%

This purity is assessed to be 99.2%.

Product Reviewed By:

James Rixson, PhD
Head of Production

Product Released By:

Jason Chaplin, PhD
Principal Chemist
Release Date: 22 December 2022

The calculation of the purity follows the formula:

$$\text{Purity}(\%) = \frac{((\text{Chromatographicpurity[HPLC]})x(100 - (\text{watercontent} + \text{ashcontent} + \text{volatilecontents})))}{100}$$

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