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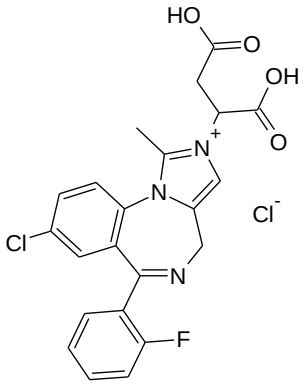
Our Formula. Your Success.

Reference Material Product Information Sheet

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



Name	8-chloro-2-(1,2-dicarboxyethyl)-6-(2-fluorophenyl)-1-methyl-4H-imidazo[1,5-a][1,4]benzodiazepin-2-ium chloride
Synonym(s)	8-chloro-2-(1,2-dicarboxyethyl)-6-(2-fluorophenyl)-1-methyl-4H-Imidazo[1,5-a][1,4]benzodiazepinium chloride
Epichem Item #	EPL-AA275 Batch 1
CAS #	2531288-23-8 (inner salt)
Molecular Formula	$C_{22}H_{18}ClFN_3O_4.Cl$
Molecular Weight	478.31 g/mol
Appearance	White solid
Melting Point	174.3-181.0°C (decomposition)
Combustion Analysis	Required (%): C:55.2; H:3.8; N:8.8. Found (%): C:53.1; H:4.0; N:8.4.
Ion Chromatography	Required (%): Cl: 7.4. Found (%) Cl: 7.2.
Purity	94.5%
Date of Manufacture	17 December 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:

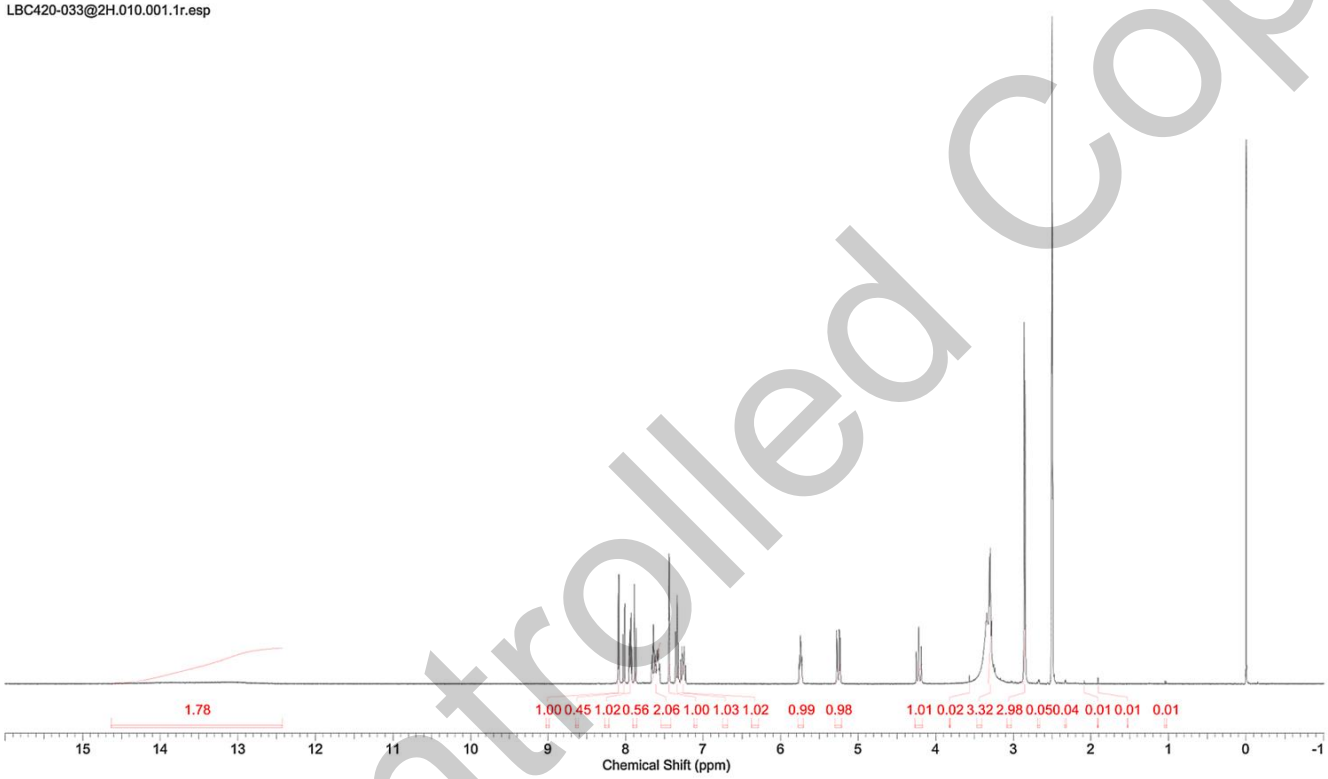
Ia. ^{1}HNMR Spectrum

Conditions: 400 MHz, DMSO-d_6

^{1}HNMR spectrum consistent with chemical structure.

Acquisition Time (sec)	3.9977	*Date*	15 Dec 2020 10:33:36		*Date Stamp*	15 Dec 2020 10:33:36	
File Name	\\naphthalene\company\NMR files\LBC420\LBC420-033@2H\10\pdata\1\1r				*Frequency (MHz)*	400.13	*Nucleus* 1H
Number of Transients	8	*Origin*	Avance	*Original Points Count* 32768	*Owner*	Walkup	*Points Count* 131072
Pulse Sequence	zg30	*Receiver Gain*	101.00	*SW(cyclical) (Hz)* 8196.72	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)* 2468.6372
Spectrum Type	STANDARD	*Sweep Width (Hz)*	8196.66	*Temperature (degree C)* 25.000			

LBC420-033@2H.010.001.1r.esp



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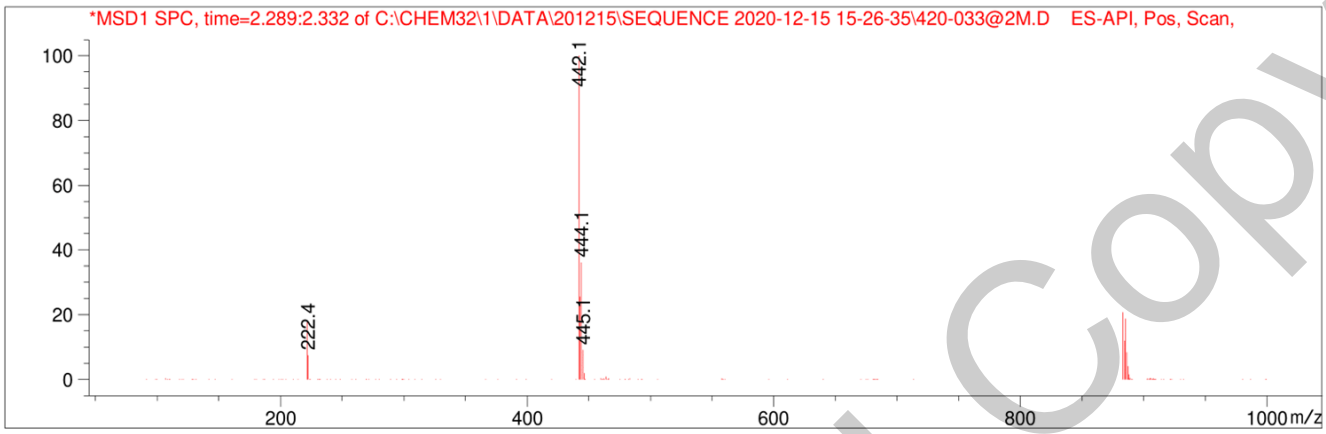
Ib. Mass Spectrum

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

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

ZORBAX SB-C8, 4.6 x 30 mm, 3.5 micron.



Theoretical value: 442.1 $[M+H]^+$.

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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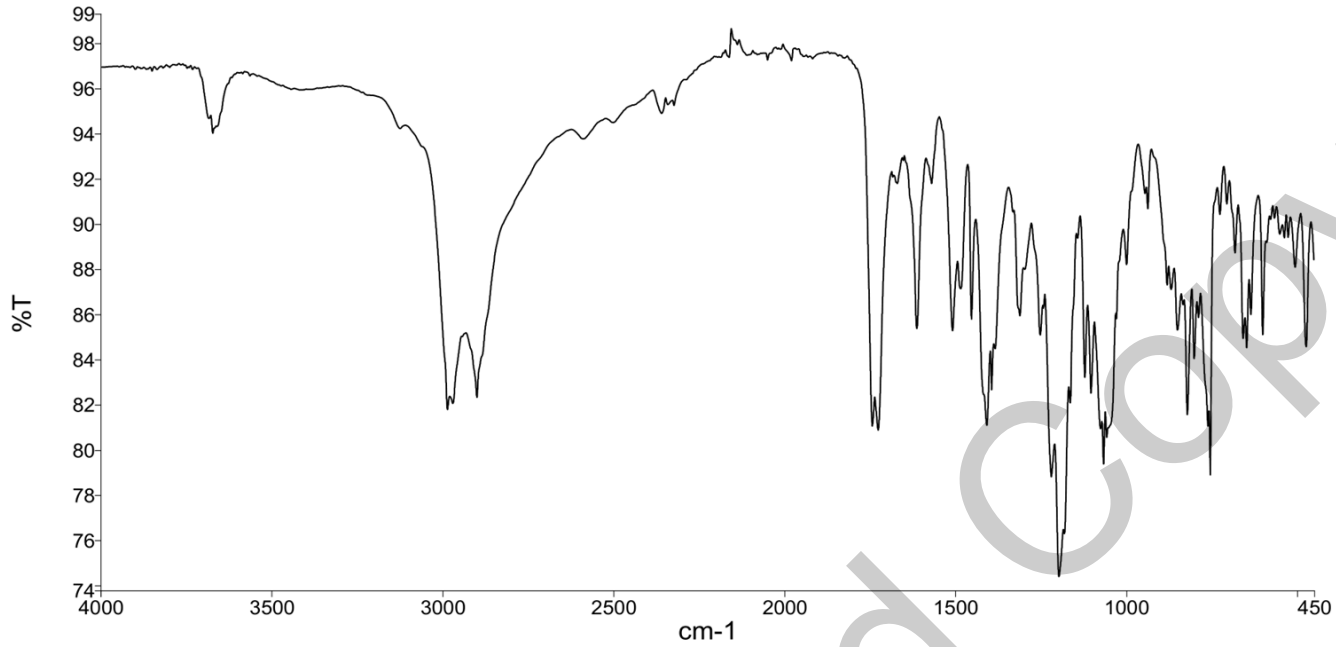
Ic. IR Spectrum

The infra-red spectrum of this material was analysed by Fourier-Transform 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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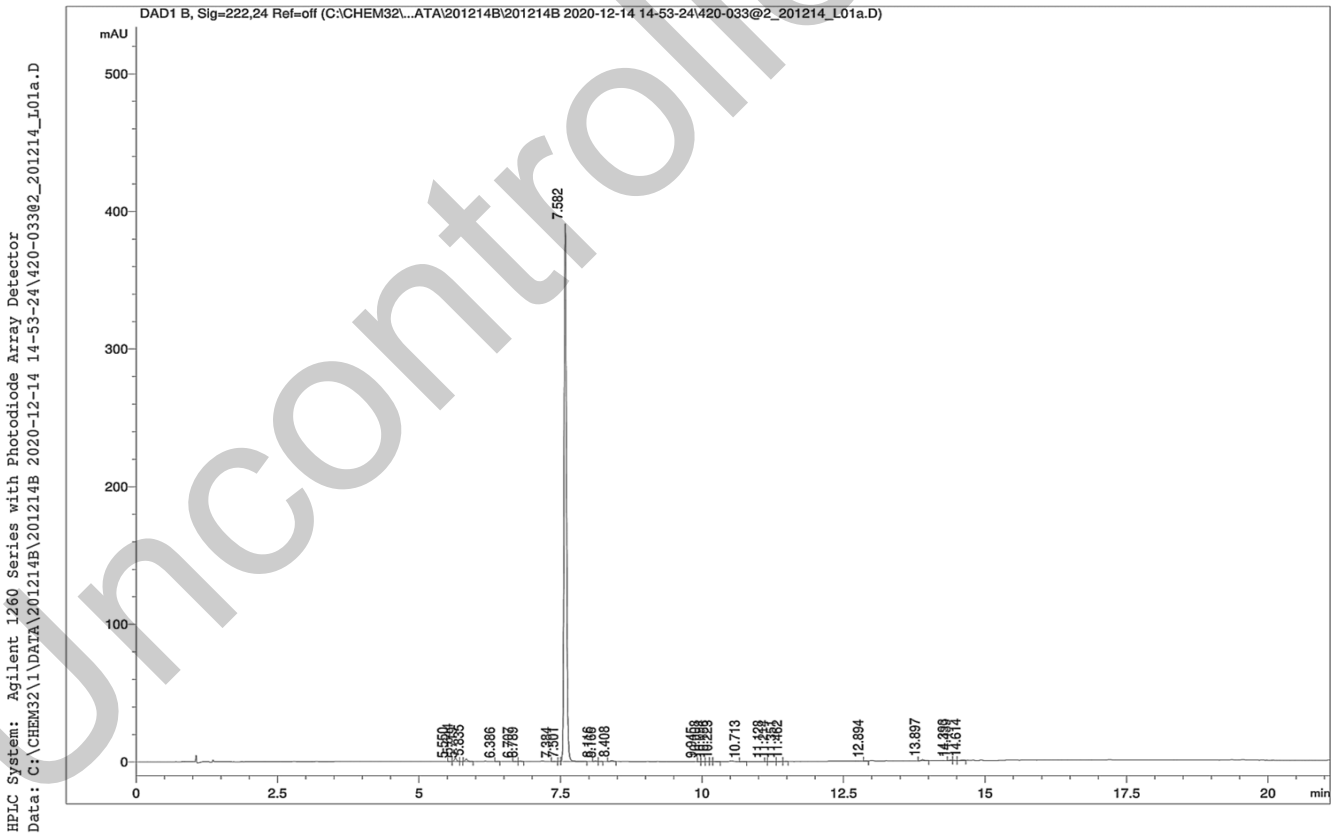
II. Purity

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

HPLC Conditions:

Column	Conditions				Detector	Injector
Agilent ZORBAX Eclipse XDB-C18 4.6 x 100mm 3.5 micron	25ºC				DAD 222nm	Auto 1.0 µL 0.35 mg/mL in 100% methanol (NO MODIFIERS)
	Time (min)	% Line A [Mixed phosphate buffer (16 mM) in water]*	% Line B [Mixed phosphate buffer (16 mM) in (v/v) 70% acetonitrile / 30% water]#	Flow rate (mL/min)		
	0.00	95	5	1.0		
	10.00	45	55	1.0		
	14.50	0	100	1.0		
	19.50	0	100	1.0		
	20.50	95	5	1.0		
	24.50	95	5	1.0		

* Contains: potassium dihydrogen phosphate (1.633 g, 12 mmol), disodium hydrogen phosphate (0.568 g, 4 mmol), water (1000 mL).
# Contains: potassium dihydrogen phosphate (1.633 g, 12 mmol), disodium hydrogen phosphate (0.568 g, 4 mmol), water (300 mL), acetonitrile (700 mL).



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Area Percent Report – Sorted by Signal

Peak Number	Retention Time (rounded)	Area	Area % (rounded)
1	5.55	0.06	0.00
2	5.64	6.34	0.54
3	5.72	0.05	0.00
4	5.83	4.38	0.37
5	6.39	0.17	0.01
6	6.71	0.10	0.01
7	6.79	0.40	0.03
8	7.38	0.07	0.01
9	7.50	0.31	0.03
10	7.58	1143.04	97.79
11	8.12	0.71	0.06
12	8.17	0.08	0.01
13	8.41	2.20	0.19
14	9.95	0.14	0.01
15	10.01	0.17	0.01
16	10.09	0.39	0.03
17	10.16	0.31	0.03
18	10.22	0.38	0.03
19	10.71	0.31	0.03
20	11.13	0.07	0.01
21	11.21	0.62	0.05
22	11.35	0.32	0.03
23	11.46	0.19	0.02
24	12.89	0.46	0.04
25	13.90	2.96	0.25
26	14.39	1.21	0.10
27	14.44	0.99	0.08
28	14.61	2.48	0.2
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 97.6% (average of 10 duplicate analyses)

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III. Water Content

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

Results:

Average 3.2%

IV. Ash Content

Method: BP2021 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)	97.6%
Water content	3.2%
Ash content	<0.1%
Residual solvents	<0.1%
Purity	94.5%

This purity is assessed to be 94.5%.

Product Reviewed By:

James Rixson, PhD
Head of Production

Product Released By:

Boon Tan
Quality Manager

Release Date: 7 April 2021

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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