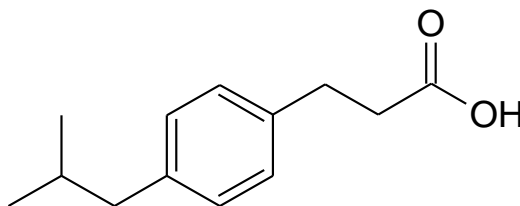


Reference Material Product Information Sheet

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



Name	3-(4-isobutylphenyl)propanoic acid
BP Name	Ibuprofen Impurity F
Synonym(s)	3-(4-isobutylphenyl)propionic acid; 3-(4-(2-methylpropyl)phenyl)propanoic acid
Epichem Item #	EPL-AA24 Batch 3
CAS #	65322-85-2
Molecular Formula	C ₁₃ H ₁₈ O ₂
Molecular Weight	206.29 g/mol
Appearance	Colourless crystals
Melting Point	63.8-66.5°C
Combustion Analysis	Required (%): C:75.7; H:8.8. Found (%): C:75.6; H:8.8.
Purity*	99.5%
Date of Manufacture	20 June 2007
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)

* NATA accreditation does not cover the performance of this service

EPL-AA24 Batch 3

Revision 3

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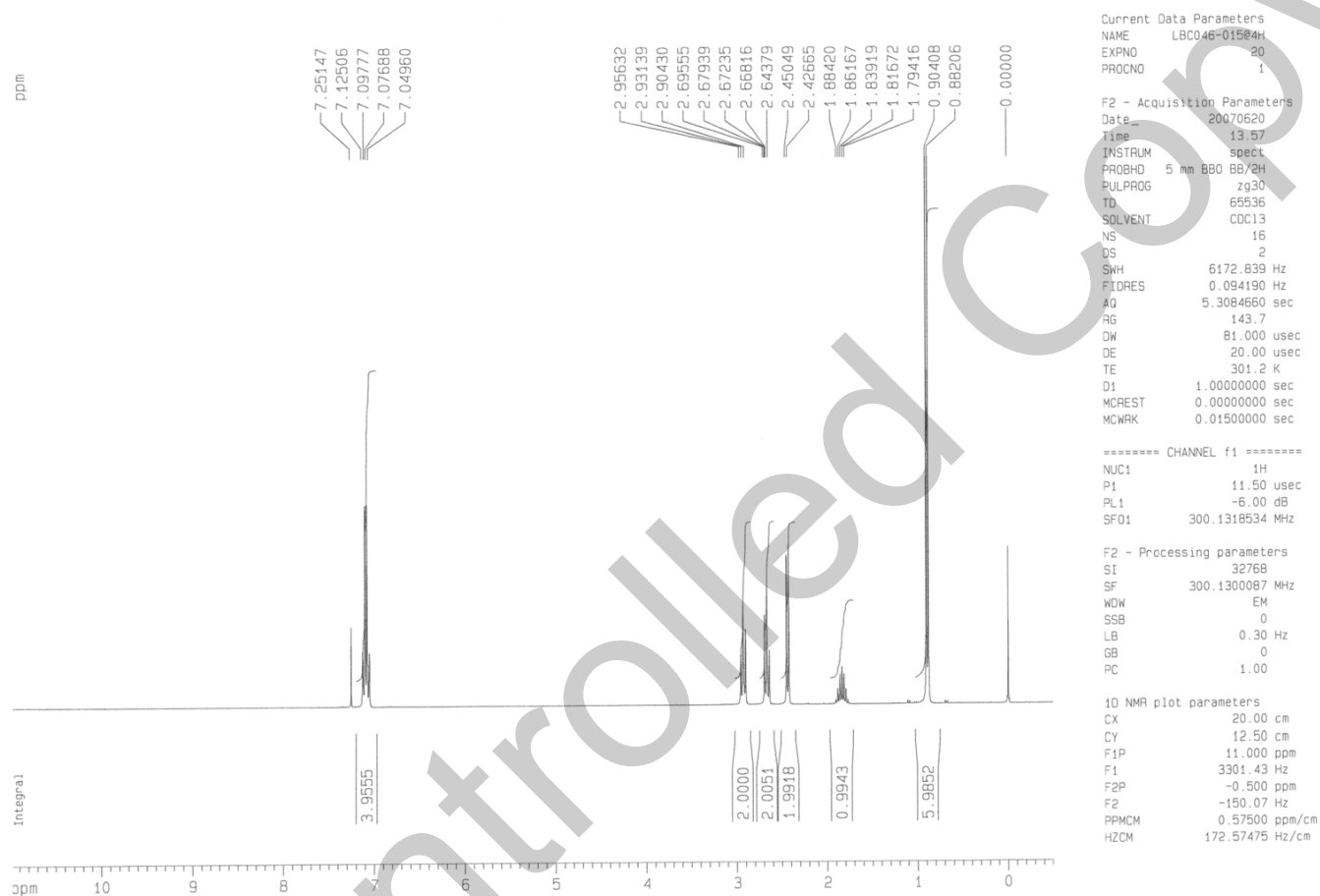
I. Identity

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

Ia. ¹HNMR Spectrum

Conditions: 300 MHz, CDCl₃

¹HNMR spectrum consistent with chemical structure.



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Revision 3

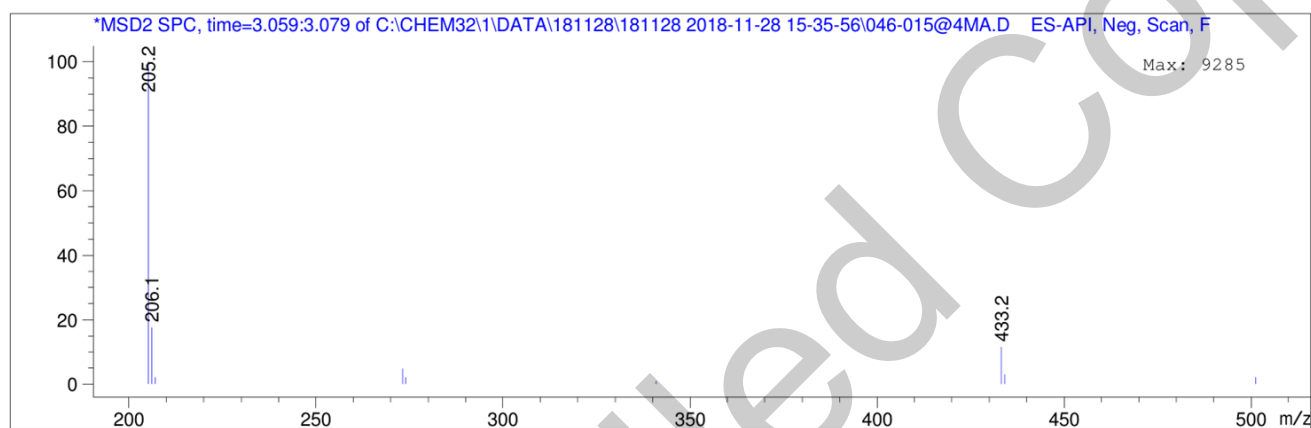
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Ib. Mass Spectrum

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
3.074	55274	433.20 I 206.10 I 205.20 I



Theoretical value: 205.2 [M-H]⁻.

The signal of the Mass Spectrum is consistent with the theoretical value and its interpretation is consistent with the structural formula.

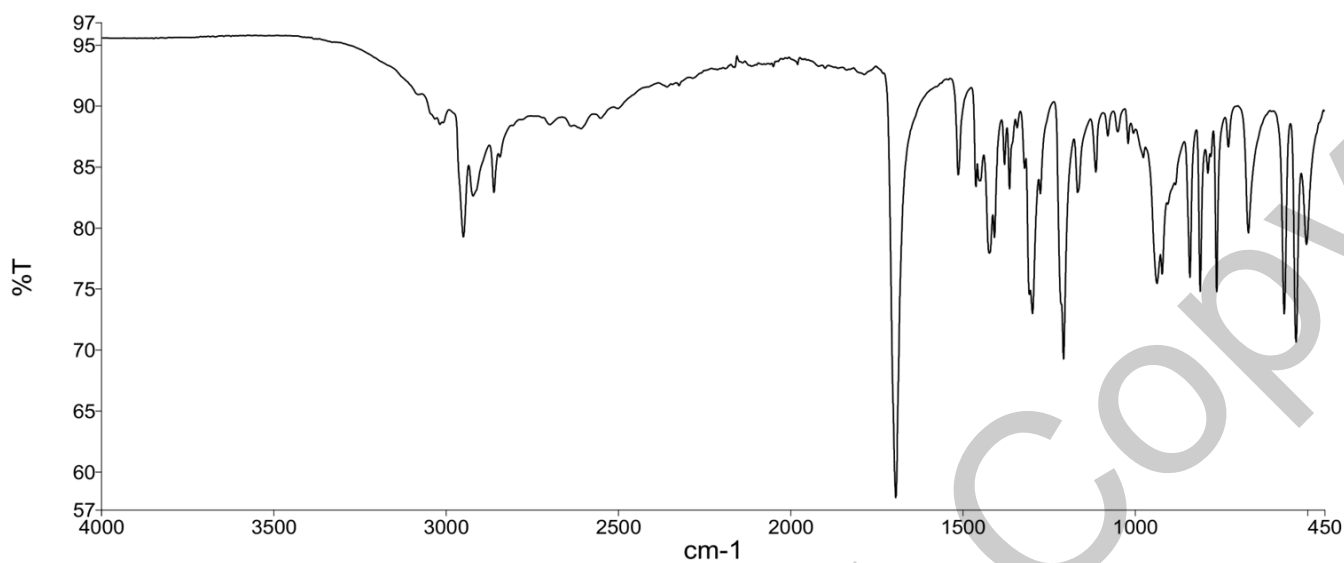
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Ic. IR Spectrum

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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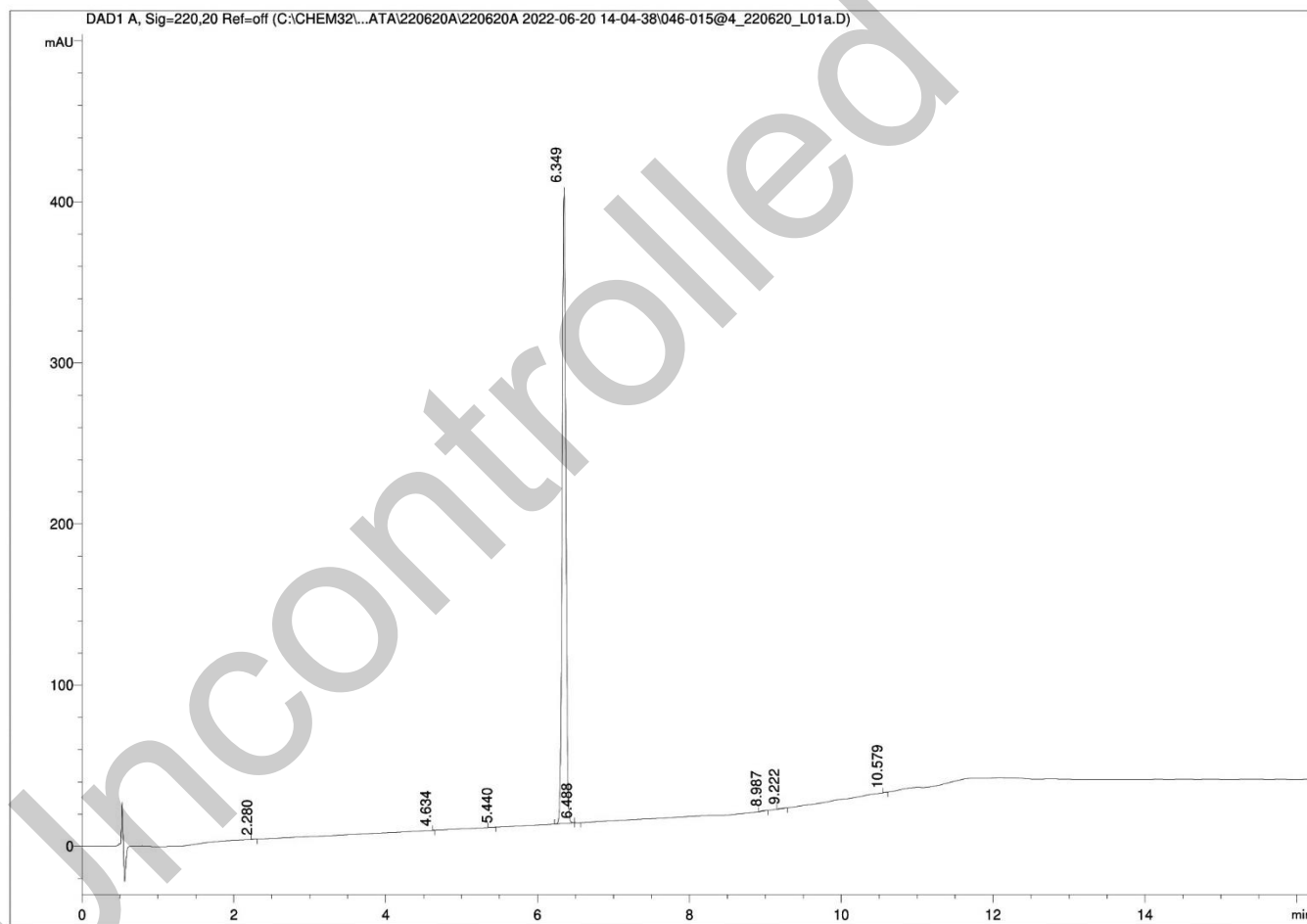
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II. Purity

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 EC-C18 4.6 x 50mm 2.7 micron	25°C				DAD 220nm	Auto 1.0 µL 0.8 mg/mL in 100% acetonitrile (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	70	30	1.0		
	7.00	35	65	1.0		
	10.00	5	95	1.0		
	15.00	5	95	1.0		
	16.00	70	30	1.0		
	19.00	70	30	1.0		



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Area Percent Report – Sorted by Signal

Peak Number	Retention Time (rounded)	Area	Area % (rounded)
1	2.28	0.27	0.02
2	4.63	0.08	0.01
3	5.44	0.24	0.02
4	6.35	1322.07	99.77
5	6.49	0.51	0.04
6	8.99	1.27	0.10
7	9.22	0.39	0.03
8	10.58	0.27	0.02
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 99.8% (average of 10 duplicate analyses)

III. Water Content

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

Results:

Average <0.1%

IV. Ash Content

Method: Ash analysis.

Result:

Contains 0.3% ash.

V. Residual Solvents

Method: ¹HNMR

Result:

No significant impurities detected by ¹H NMR analysis.

VI. Final Result

Chromatographic purity (HPLC)	99.8%
Water content	<0.1%
Ash content	0.3%
Residual solvents	<0.1%
Purity*	99.5%

This purity is assessed to be 99.5%.

Product Reviewed By:

Product Released By:

James Rixson, PhD
Head of Production

Carol Worth, PhD
Quality Manager

Release Date: 23 June 2022

*NATA accreditation does not cover the performance of this service.
The calculation of the purity follows the formula:

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

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