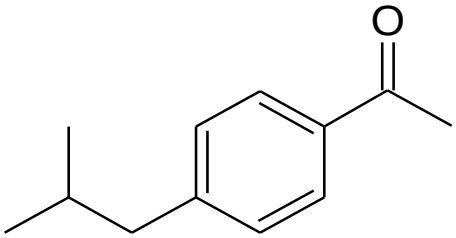
Our Formula. Your Success.

Reference Material Product Information Sheet

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



Name	4'-isobutylacetophenone
BP Name	Ibuprofen Impurity E
Synonym(s)	1-(4-(2-methylpropyl)phenyl)ethanone
Epichem Item #	EPL-AA22 Batch 1
CAS #	38861-78-8
Molecular Formula	$C_{12}H_{16}O$
Molecular Weight	176.26 g/mol
Appearance	Colourless liquid
Combustion Analysis	Required (%): C:81.8; H:9.2. Found (%): C:81.7; H:9.1.
Purity	97.7%
Date of Manufacture	15 May 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)

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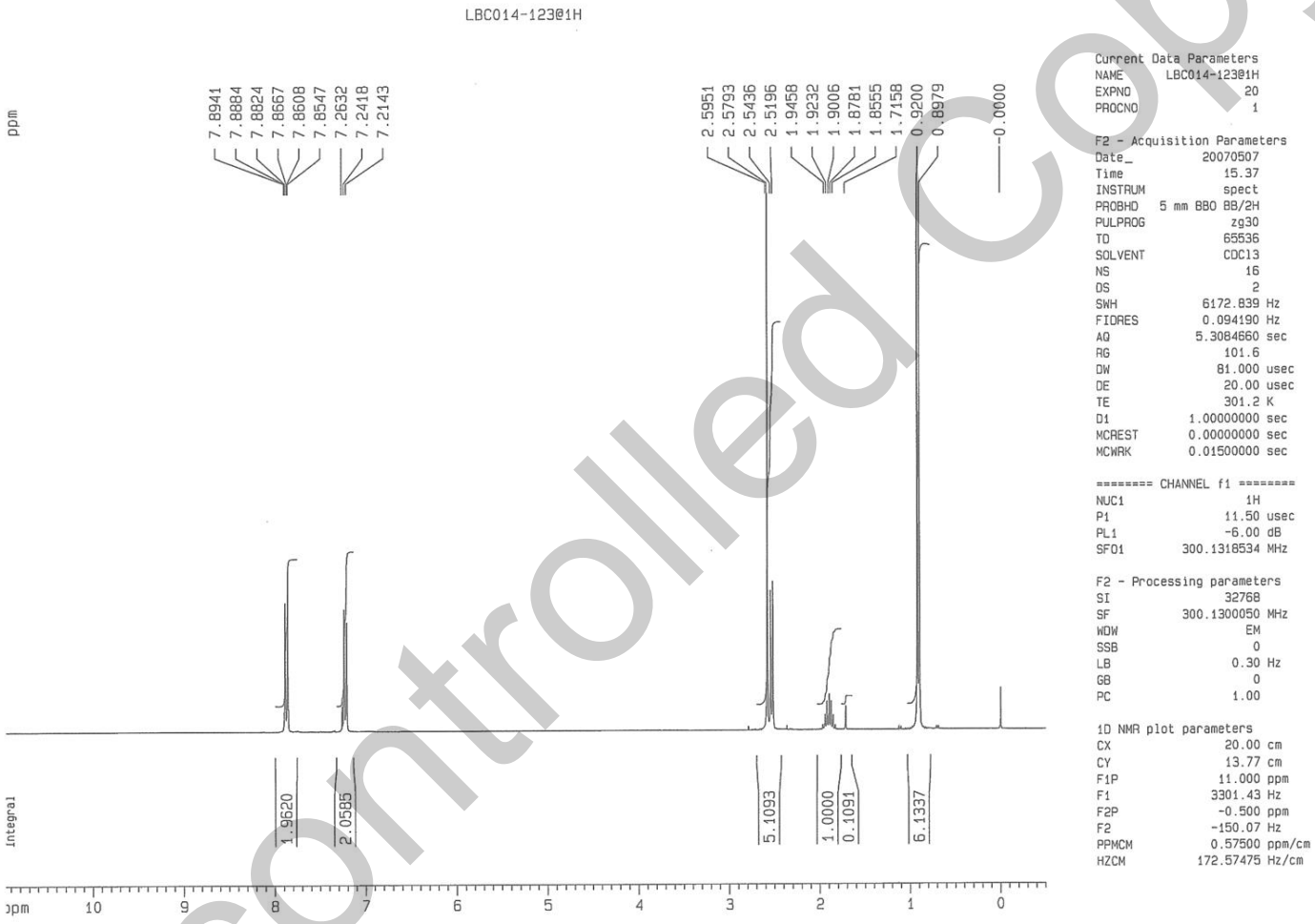
I. Identity

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

Ia. [1]HNMR Spectrum

Conditions: 300 MHz, $CDCl_3$

[1]HNMR spectrum consistent with chemical structure.



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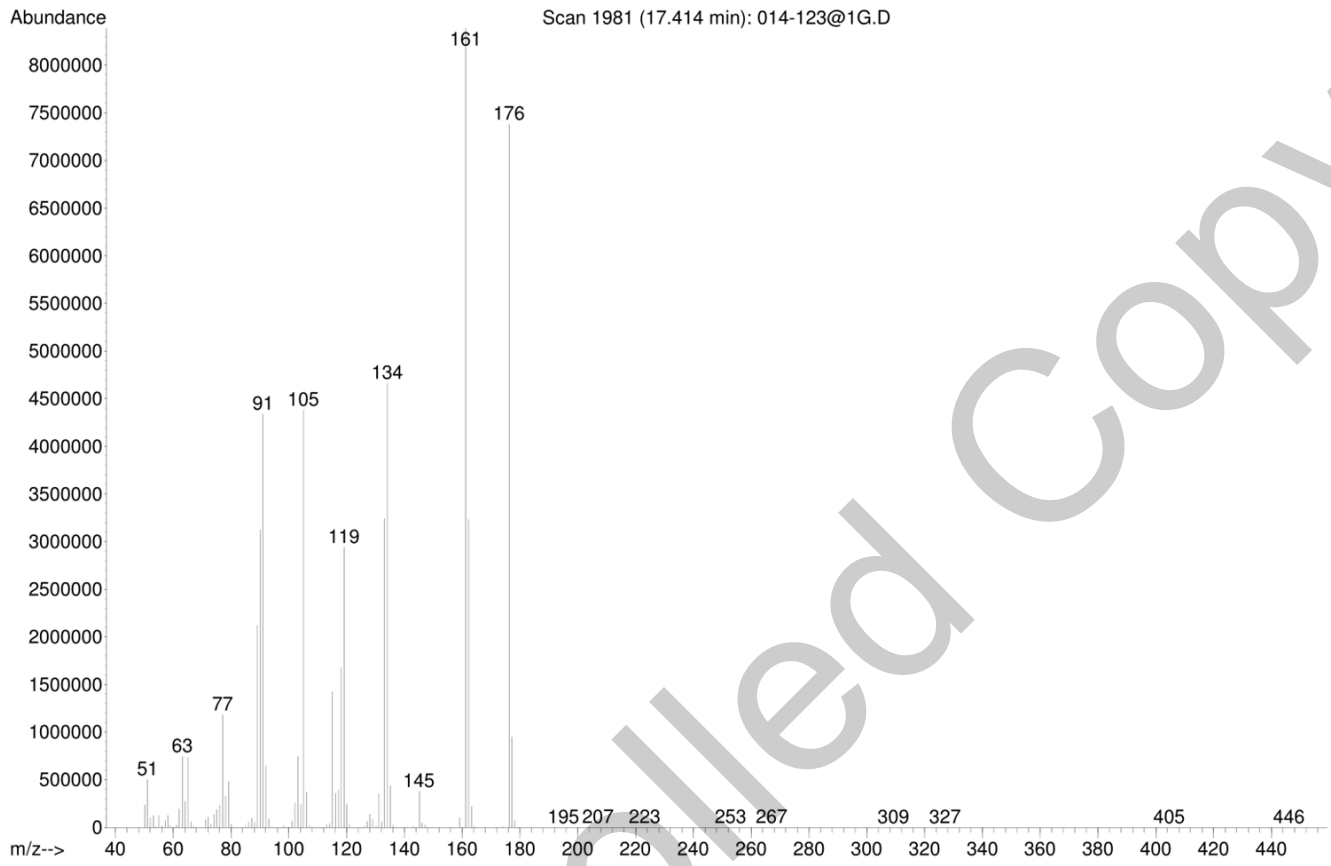
Ib. Mass Spectrum

The mass spectrum of this material was analysed by Gas chromatography–mass spectrometry (GCMS).

Method: Agilent HP-5MS column; 30 m x 0.25mm, 0.25 micron



Theoretical values: 176 $[M]^{+\cdot}$

The signals of the Mass Spectrum are consistent with the theoretical value and their interpretation is consistent with the structural formula.

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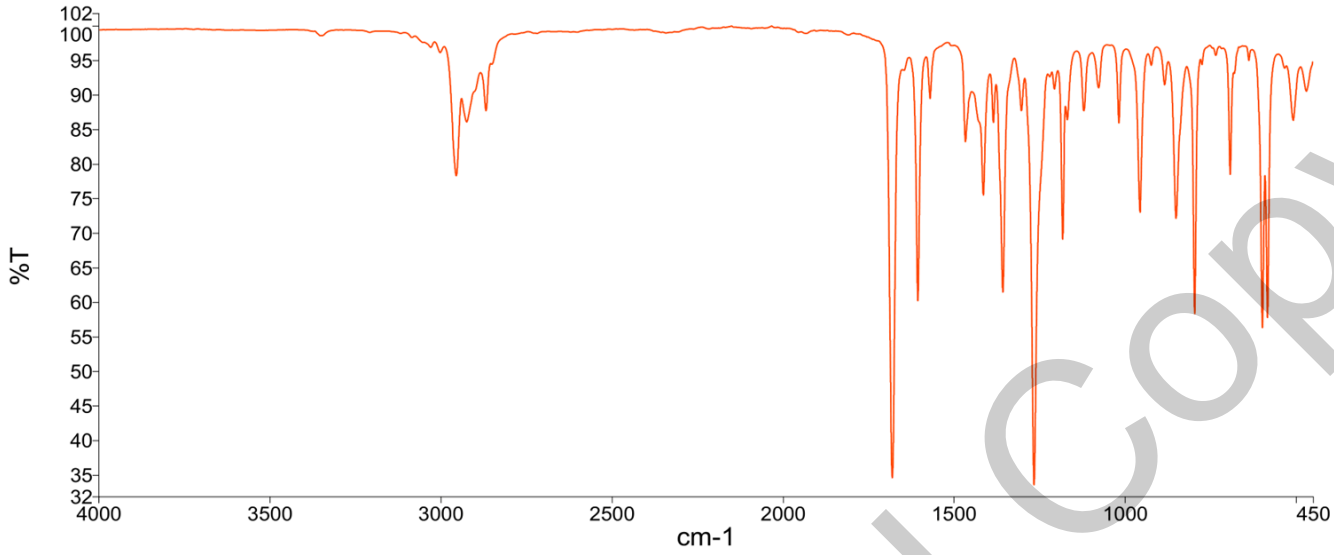
Ic. IR Spectrum

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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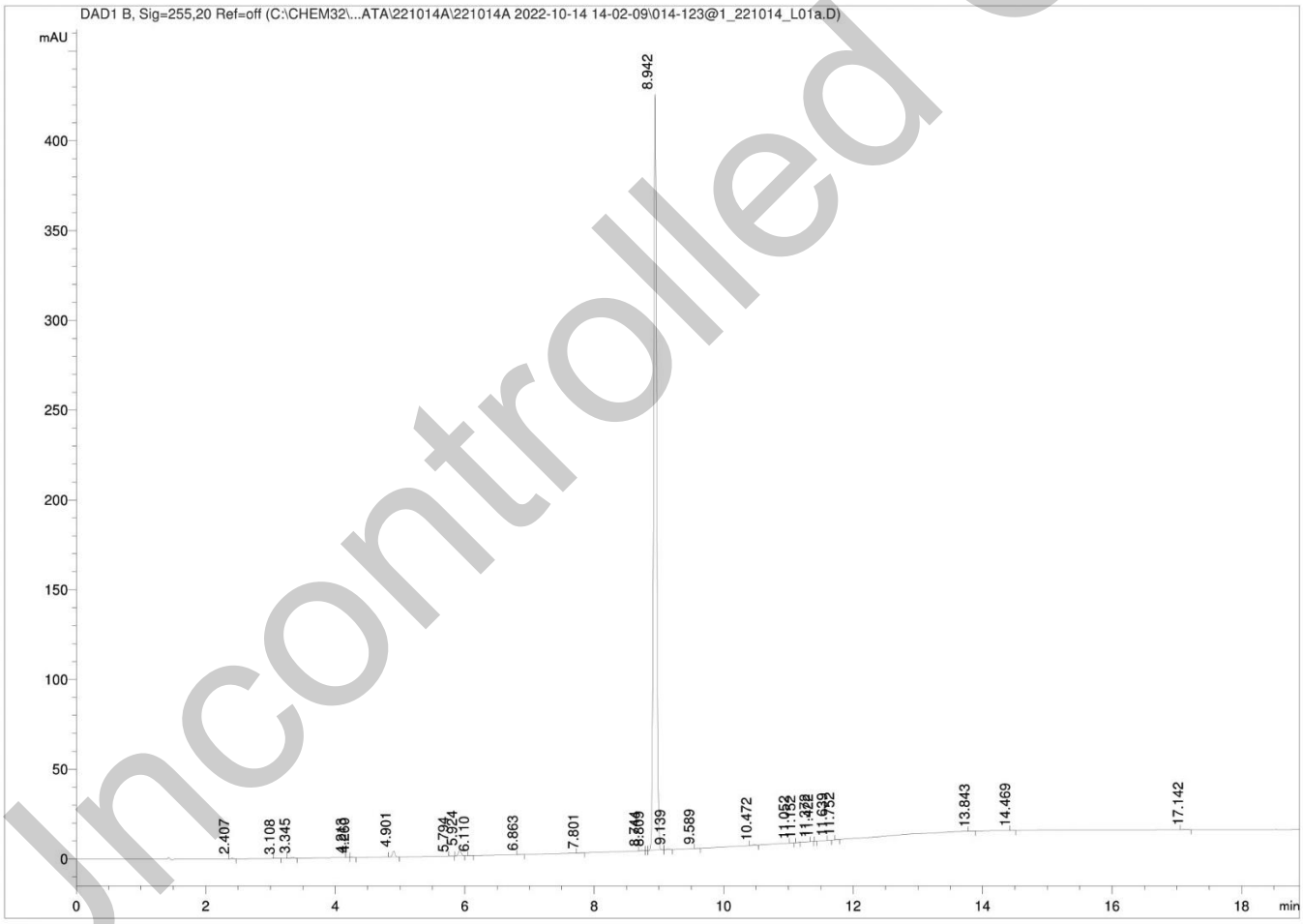
II. Purity

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 EC-C18 4.6 x 150 mm 2.7 micron	25ºC				DAD 255nm	Auto 1.0 µL 0.3mg/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	60	40	1.0		
	11.00	5	95	1.0		
	17.00	5	95	1.0		
	18.00	60	40	1.0		
	27.00	60	40	1.0		



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Area Percent Report – Sorted by Signal

Peak Number	Retention Time (rounded)	Area	Area % (rounded)
1	2.41	0.96	0.07
2	3.11	0.20	0.01
3	3.34	1.59	0.11
4	4.21	0.40	0.03
5	4.26	1.04	0.07
6	4.90	8.98	0.64
7	5.79	0.08	0.01
8	5.92	9.83	0.70
9	6.11	0.08	0.01
10	6.86	0.15	0.01
11	7.80	0.30	0.02
12	8.74	0.58	0.04
13	8.81	0.06	0.00
14	8.94	1372.72	97.9
15	9.14	1.71	0.12
16	9.59	0.12	0.01
17	10.47	1.26	0.09
18	11.05	0.05	0.00
19	11.15	0.07	0.01
20	11.37	0.05	0.00
21	11.42	0.02	0.00
22	11.64	0.06	0.00
23	11.75	0.06	0.00
24	13.84	0.25	0.02
25	14.47	0.19	0.01
26	17.14	1.31	0.09
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 97.9% (average of 10 duplicate analyses)

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III. Water Content

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

Results:

Average 0.2%

IV. Ash Content

Method: Combustion adjuvant added.

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)	97.9%
Water content	0.2%
Ash content	<0.1%
Residual solvents	<0.1%
Purity	97.7%

This purity is assessed to be 97.7%.

Product Reviewed By:

James Rixson, PhD
Head of Production

Product Released By:

Carol Worth, PhD
Quality Manager

Release Date: 31 October 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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