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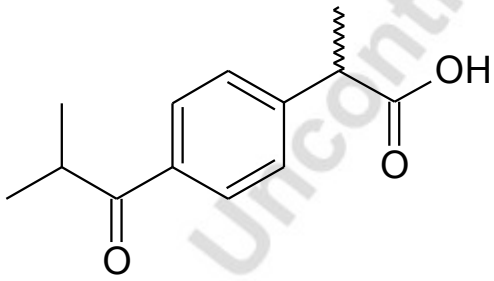
# Reference Material Product Information Sheet

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




| | |
|---|---|
| **Name** | (*RS*)-2-(4-isobutyrylphenyl)propanoic acid |
| **BP Name** | Ibuprofen Impurity J |
| **Synonym(s)** | (*RS*)-2-(4-isobutyrylphenyl)propionic acid;<br>(2*RS*)-2-(4-(2-methyl-propanoyl)phenyl)propanoic acid |
| **Epichem Item #** | EPL-AA23 Batch 6 |
| **CAS #** | 65813-55-0 |
| **Molecular Formula** | $C_{13}H_{16}O_3$ |
| **Molecular Weight** | 220.27 g/mol |
| **Appearance** | Off-white powder |
| **Melting Point** | 86.2-89.0°C |
| **Combustion Analysis** | Required (%): C:70.9; H:7.3; N:0.0. Found (%): C:70.9; H:7.3; N:0.0. |
| **Purity*** | 99.3% |
| **Date of Manufacture** | 13 August 2010 |
| **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*



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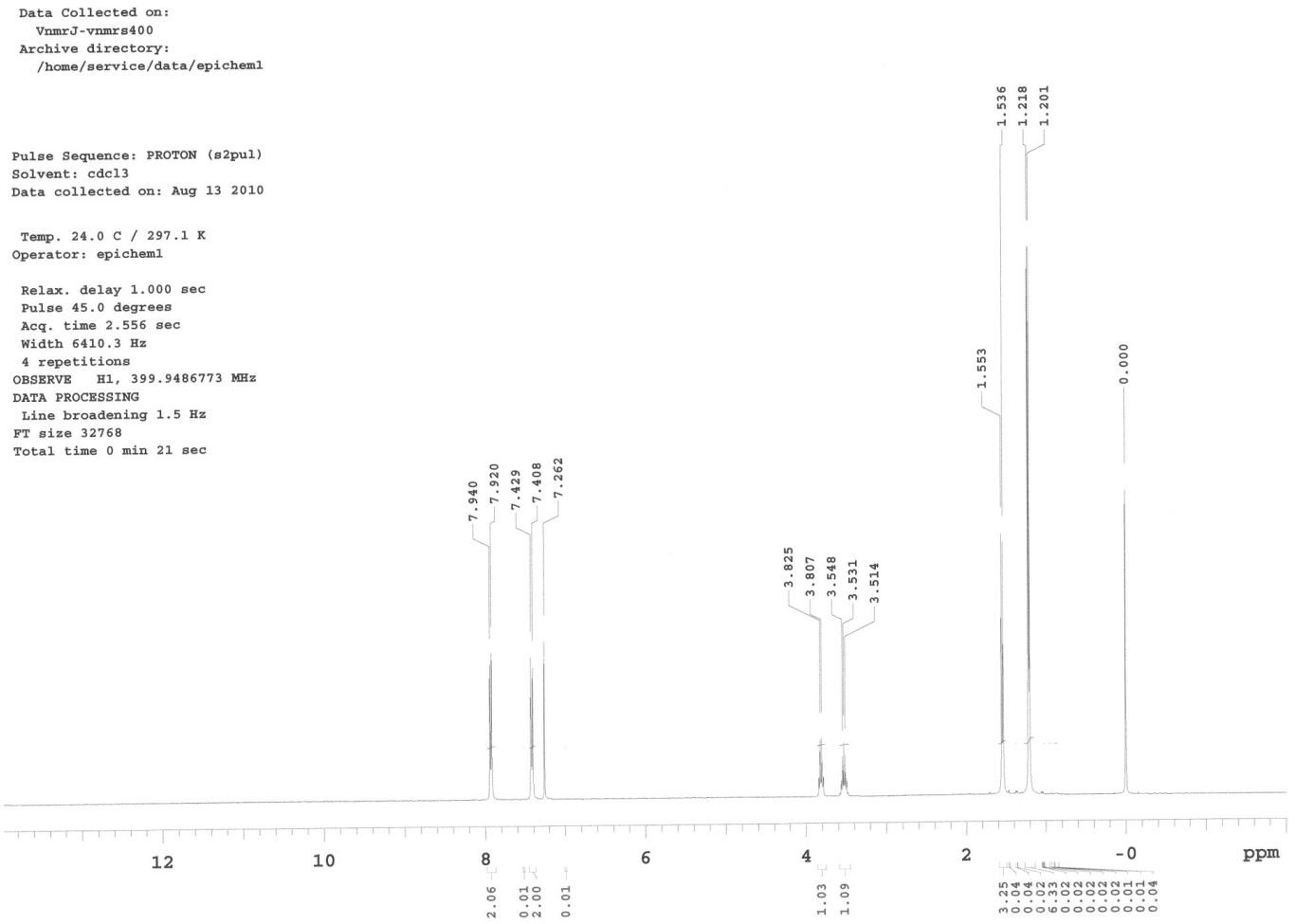
## I. Identity

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

### Ia. $^{1}$HNMR Spectrum

Conditions: 400 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 Liquid Chromatography Mass Spectroscopy (LCMS) using in-house EM005.WI08.

Method: 20-100% ACN in water gradient (+0.1% formic acid)

Agilent Poroshell 120 SB-C8, 2.1 x 100, 2.7 micron


Theoretical value: 221.2 $[M+H]^+$.

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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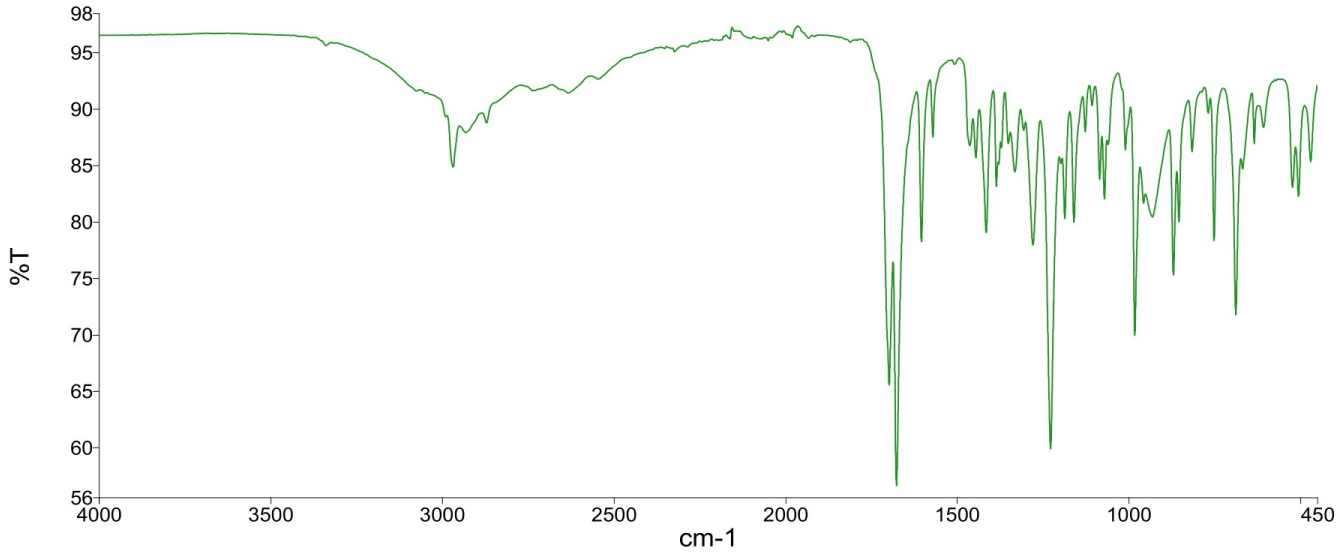
## Ic. IR Spectrum

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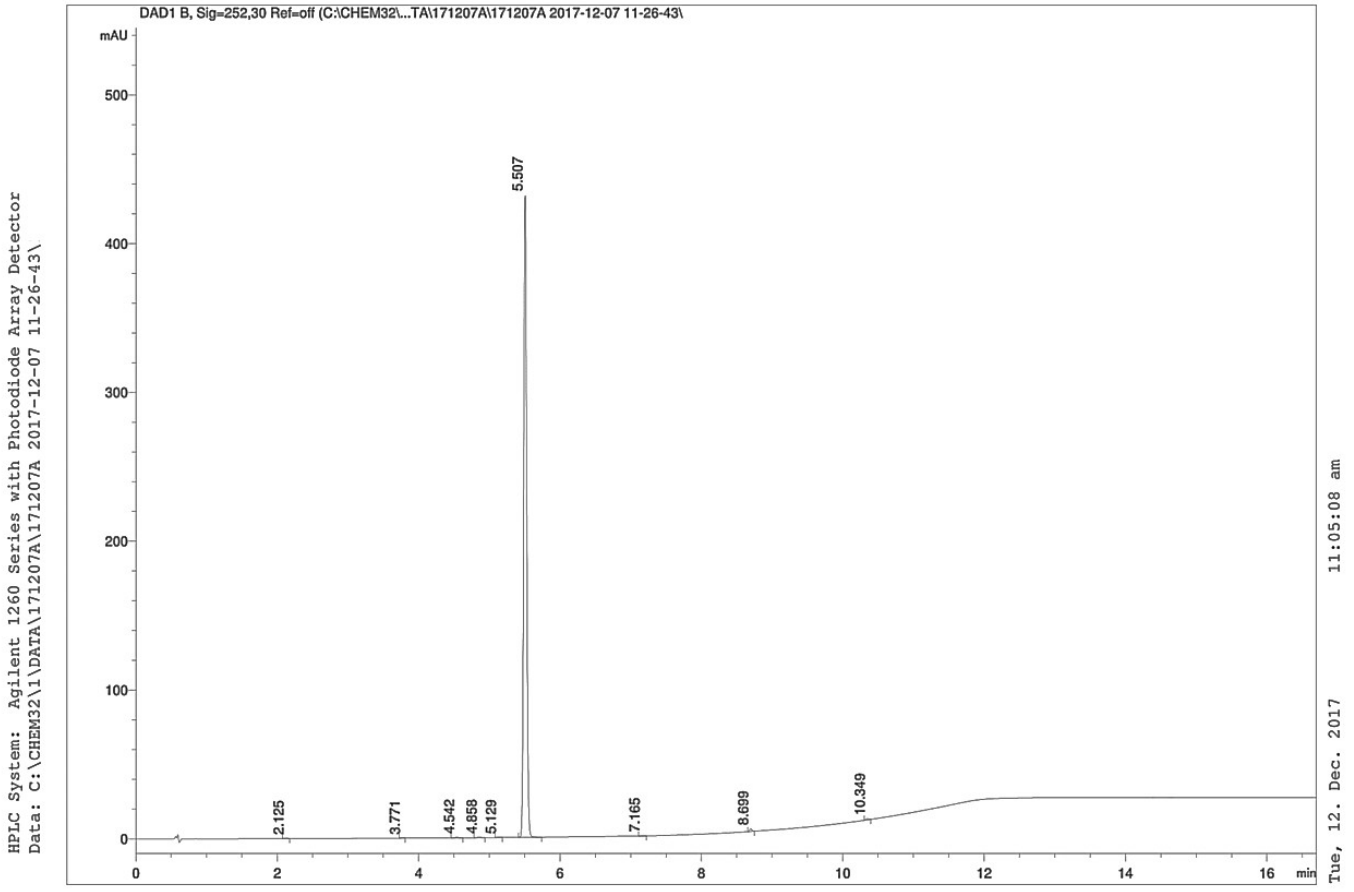
## II. Purity

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 Poroshell 120 EC-C18<br><br>4.6 x 50mm<br><br>2.7 micron | 25ºC | | | | DAD<br><br>252nm | Auto<br><br>1.0 µL<br><br>0.4 mg/mL 100% acetonitrile |
| | Time (min) | % Line A (Water + 0.1% (v/v) TFA) | % Line B (Acetonitrile + 0.1% (v/v) TFA) | Flow rate (mL/min) | | |
| | 0.00 | 80 | 20 | 1.0 | | |
| | 6.00 | 50 | 50 | 1.0 | | |
| | 10.50 | 5 | 95 | 1.0 | | |
| | 15.50 | 5 | 95 | 1.0 | | |
| | 16.50 | 80 | 20 | 1.0 | | |
| | 19.50 | 80 | 20 | 1.0 | | |



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**Area Percent Report – Sorted by Signal**

| Peak Number | Retention Time (rounded) | Area | Area % (rounded) |
|---|---|---|---|
| 1 | 2.13 | 0.40 | 0.03 |
| 2 | 3.77 | 0.16 | 0.01 |
| 3 | 4.54 | 1.43 | 0.11 |
| 4 | 4.86 | 0.96 | 0.08 |
| 5 | 5.13 | 0.28 | 0.02 |
| 6 | 5.51 | 1244.73 | 99.27 |
| 7 | 7.17 | 0.46 | 0.04 |
| 8 | 8.70 | 3.77 | 0.30 |
| 9 | 10.35 | 1.73 | 0.14 |
| Totals | | 1253.92 | 100.00 |

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 99.3% (average of 8 duplicate analyses)





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## III. Water Content

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

**Results:**

Average <0.1%

## IV. Ash Content

Method: BP2010 Ash

**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) | 99.3% |
| Water content | <0.1% |
| Ash content | <0.1% |
| Residual solvents | <0.1% |
| Purity* | 99.3% |

This purity is assessed to be 99.3%.

Product Reviewed By:

John Moursounidis, PhD
Head Reference Standards

Product Released By:

Boon Tan
Quality Manager

Release Date: 16 July 2018

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The calculation of the purity follows the formula:

$$\text{Purity}(\%) = \frac{((\text{Chromatographic purity}[\text{HPLC}]) \text{ x } (100 - (\text{water content} + \text{ash content} + \text{volatile contents})))}{100}$$



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