



Certificate of Analysis

ISO 9001

Reference Material

Product name

(4-Methoxyphenyl)acetonitrile

Product code

MM0393.15-0100

CAS number

104-47-2

Molecular weight

147.17

Molecular formula

C₉H₉NO

Lot number

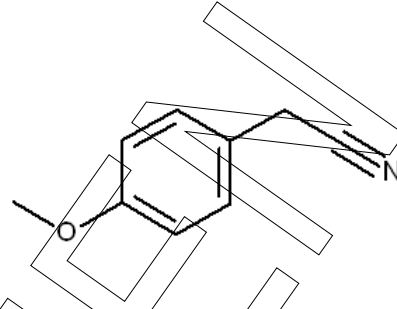
1165018

Appearance

colourless liquid

Long-term storage

2 to 8 °C, dark



Assay "as is"
99.6 %

Date of shipment:

05 Nov 2021

Producer confirms that this reference material (RM) meets the specification detailed on this Certificate of Analysis for **one year** from the date of shipment, provided the substance is stored under the recommended conditions unopened in the original container.

| | | | |
|---------------------|--------------------------|--|-----------------|
| Release by: | Date of Release: | | Product Release |
| Dr. Sabine Schröder | Luckenwalde, 17 Aug 2021 | | |



Mikromol™

Product information

For laboratory use only. Not suitable for human or animal consumption.

Before usage of the RM, it should be allowed to warm to room temperature. No drying required, as the certified value is already corrected for the content of water and other volatile materials.

The product quality is controlled by regularly performed quality control tests (retests).

Further content

Identity

Assay

Final result

Revision table

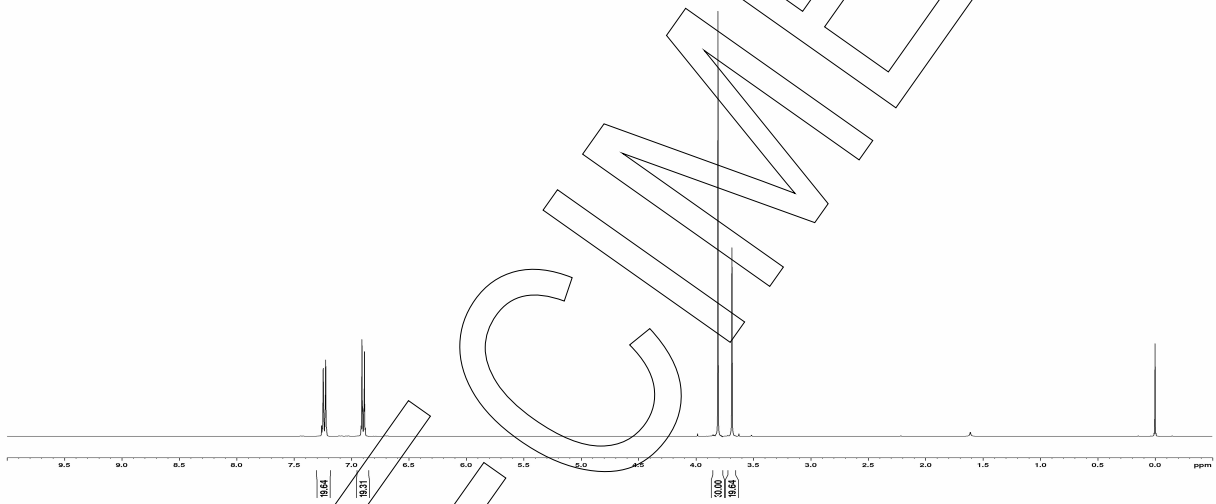
SPECIMEN



Identity

The identity of the reference material was established by following analyses.

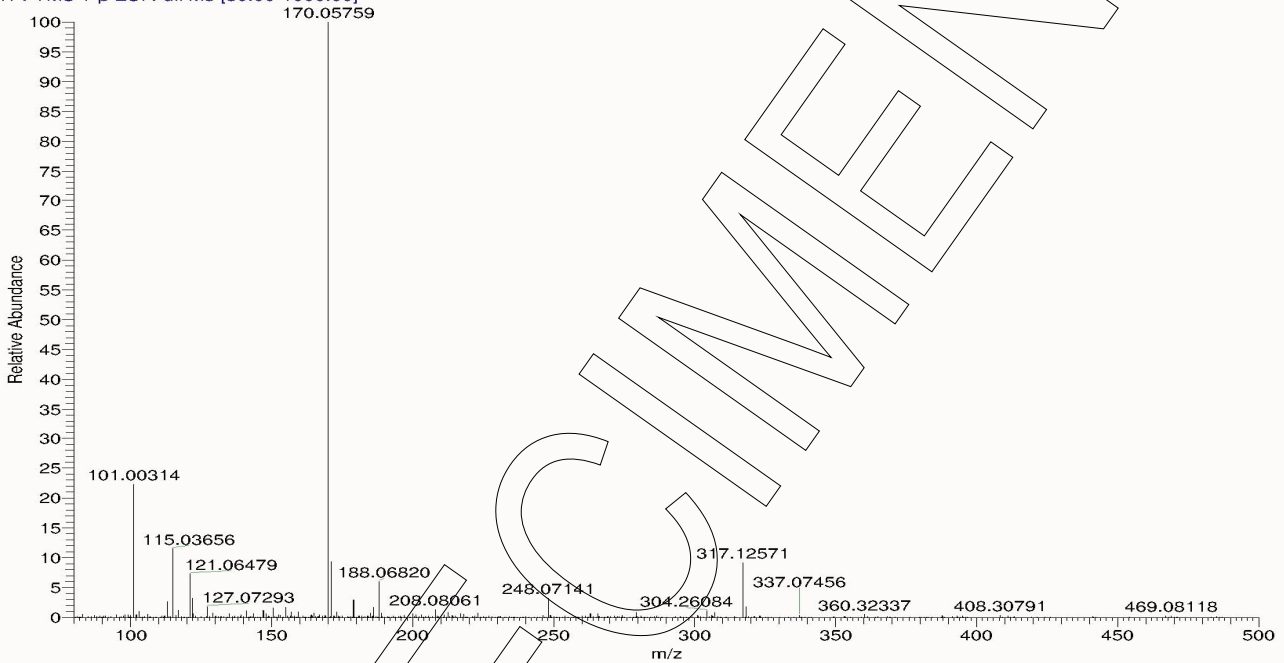
| Method | Conditions | Result |
|--------------------|----------------------------|---------------------|
| ¹ H-NMR | 400 MHz, CDCl ₃ | Structure confirmed |





| Method | Conditions | Result |
|--------|--|---------------------|
| MS | 3.5 kV ESI+; capillary temperature: 269 °C Theoretical value: 170.05764 | Structure confirmed |

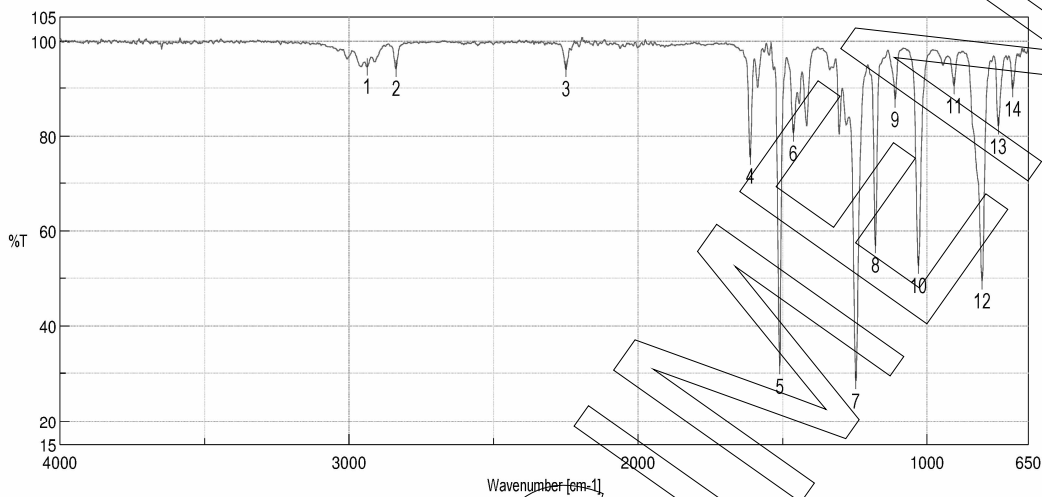
117153 #1-224 RT: 0.00-1.00 AV: 224 NL: 2.72E7
T: FTMS + p ESI Full ms [80.00-1000.00]



SPECIMEN



| Method | Conditions | Result |
|--------|--|---------------------|
| IR | Attenuated Total Reflection Fourier Transform Infrared (ATR-FTIR) Spectroscopy | Structure confirmed |



| No. | Position | Intensity |
|-----|----------|-----------|
| 1 | 2938.02 | 94.6134 |
| 2 | 2837.74 | 94.1774 |
| 3 | 2249.56 | 94.0751 |
| 4 | 1612.2 | 75.6138 |
| 5 | 1509.99 | 31.5215 |
| 6 | 1462.74 | 80.5662 |
| 7 | 1246.75 | 28.4521 |
| 8 | 1179.26 | 56.8567 |
| 9 | 1110.8 | 87.6562 |
| 10 | 1030.77 | 52.5826 |
| 11 | 907.344 | 90.4898 |
| 12 | 809.956 | 49.372 |
| 13 | 754.031 | 82.0497 |
| 14 | 703.89 | 89.8535 |



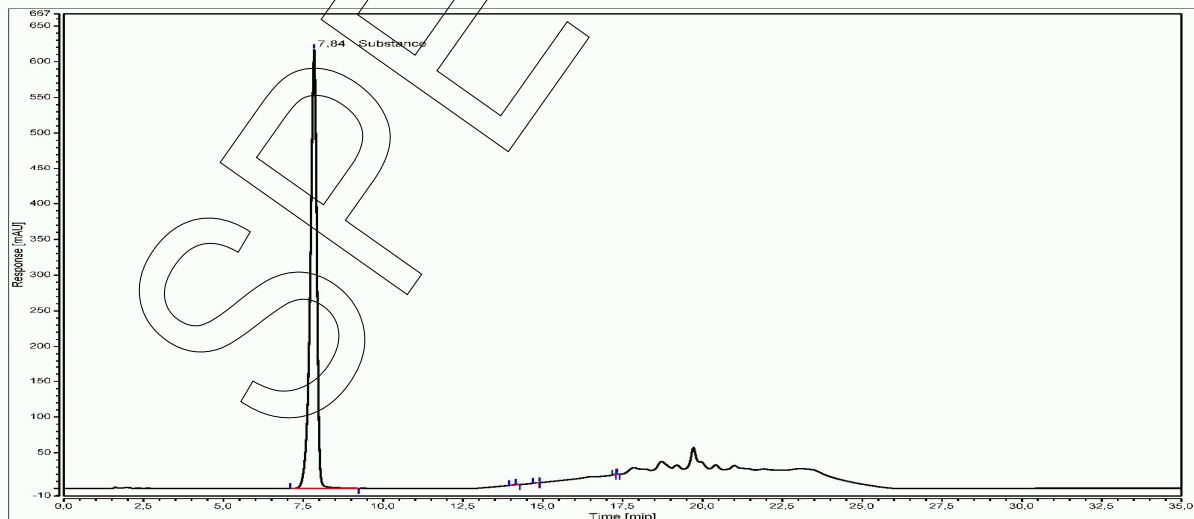
Assay

The assay of the reference material was assessed by following analyses.

Purity by high performance liquid chromatography (HPLC)

| HPLC Conditions: | |
|--------------------|--|
| Column | Hypersil Gold C18; 5 μ m, 150 x 4.6 mm |
| Column temperature | 40 °C |
| Detector | DAD, 225 nm |
| Injector | Auto 2 μ l; 0.2222 mg/ml in Acetonitrile |
| Flow rate | 1.0 ml/min |
| Phase A | Water, 0.1 % H ₃ PO ₄ |
| Phase B | Acetonitrile, 0.1 % H ₃ PO ₄ |
| Gradient program | 0-10 min A/B 70/30 10-15 min A/B to 20/80 15-20 min A/B 20/80 20-23 min A/B to 70/30 23-35 min A/B 70/30 (v/v) |

HPLC chromatogram and peak table





Area percent report - sorted by signal

| Pk # | Retention time | Area | Area % |
|---------------|----------------|-----------------|---------------|
| 1 | 7.836 | 144.7796 | 99.78 |
| 2 | 14.156 | 0.1831 | 0.13 |
| 3 | 14.896 | 0.0188 | 0.01 |
| 4 | 17.282 | 0.0545 | 0.04 |
| 5 | 17.329 | 0.0631 | 0.04 |
| Totals | | 145.0991 | 100.00 |

The content of the analyte was determined as ratio of the peak-area of the analyte and the cumulative areas of the purities, added up to 100 %. System peaks were ignored in calculation.

Result (n = 3) 99.77 %; SD = 0.02 %

Volatile content

Water content

Method Karl Fischer titration
Result (n = 3) 0.21 %; SD = 0.02 %

Residual solvents

Method ¹H-NMR
Result (n = 1) No significant amounts of residual solvents were detected (< 0.05 %).



Final result

Assay "as is": 99.56 %

The assay "as is" is assessed by 100% method (mass balance) and is equivalent to the assay based on the not anhydrous and not dried substance respectively.

The calculation of the 100% method follows the formula:

$$\text{Assay (\%)} = (100\% - \text{volatile contents (\%)}) * \frac{\text{Purity (\%)}}{100\%}$$

Volatile contents are considered as absolute contributions and purity is considered as relative contribution. Inorganic residues are excluded by additional tests.

Revision table

| Revision | Date | Reason for revision |
|----------|-------------|--|
| 00 | 17 Aug 2021 | Release of the Certificate of Analysis - initial version |

Product warranties for the RM are set out in the terms and conditions of purchase.