



# Certificate of Analysis

ISO 9001

## Reference Material

### Product name

N-[4-Cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methylpropanamide

### Product code

MM0894.01-0025

### CAS number

945419-64-7

### Molecular weight

414.37

### Molecular formula

C<sub>18</sub>H<sub>14</sub>F<sub>4</sub>N<sub>2</sub>O<sub>3</sub>S

### Lot number

1023292

### Appearance

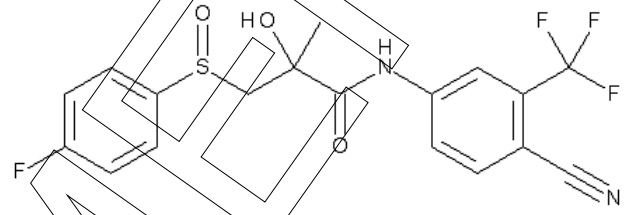
white solid

### Melting point

157 °C

### Long-term storage

2 to 8 °C, dark  
hygroscopic



Assay "as is"  
98.8 %

Date of shipment:

**13 Sep 2019**

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

|                     |                          |  |                 |
|---------------------|--------------------------|--|-----------------|
| <b>Release by:</b>  | <b>Date of Release:</b>  |  | Product Release |
| Dr. Sabine Schröder | Luckenwalde, 04 Sep 2019 |  |                 |



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

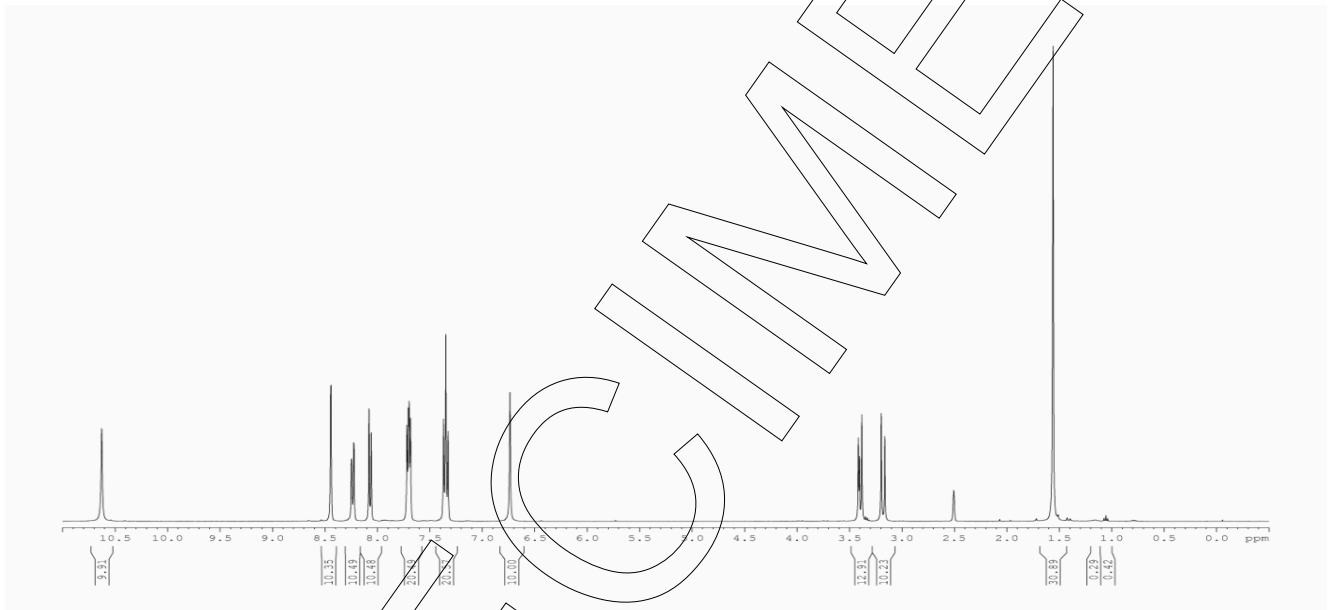
SPECIMEN



### Identity

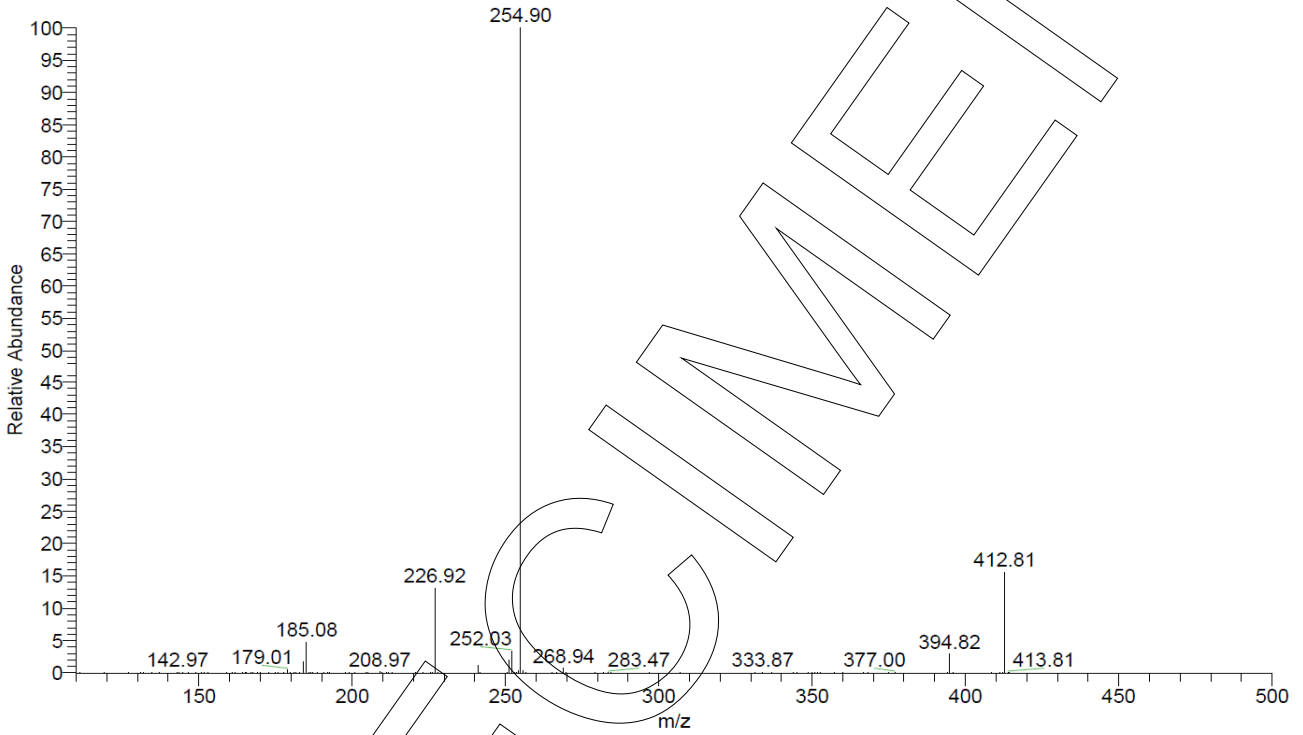
The identity of the reference material was established by following analyses.

| Method             | Conditions                   | Result              |
|--------------------|------------------------------|---------------------|
| <sup>1</sup> H-NMR | 400 MHz, DMSO-d <sub>6</sub> | Structure confirmed |





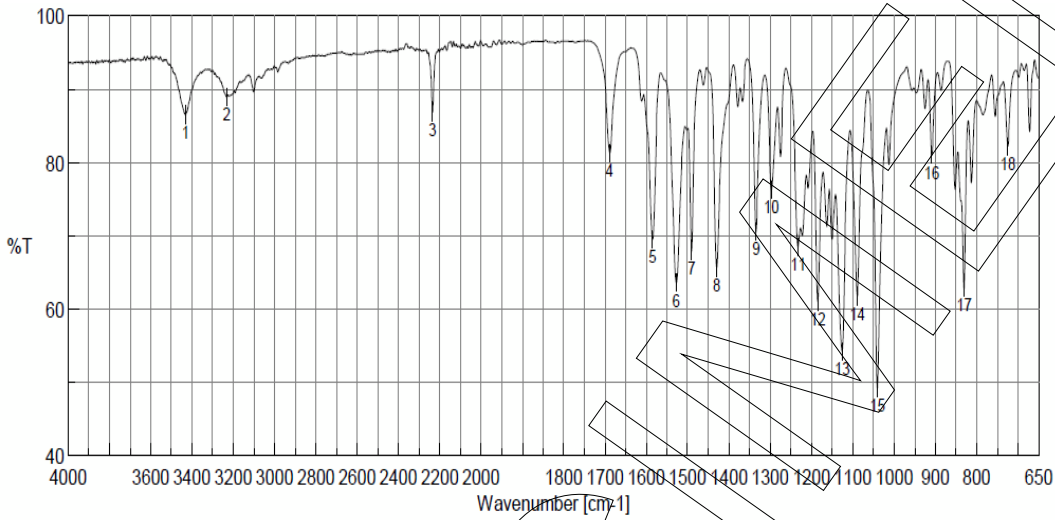
| Method | Conditions                                    | Result              |
|--------|---|---------------------|
| MS     | 4.5 kV ESI-; vaporization temperature: 200 °C | Structure confirmed |



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



| Result of Peak Picking |          |           |
|------------------------|----------|-----------|
| No.                    | Position | Intensity |
| 1                      | 3431.71  | 86.5387   |
| 2                      | 3232.11  | 88.9334   |
| 3                      | 2235.09  | 86.8436   |
| 4                      | 1688.37  | 81.3207   |
| 5                      | 1585.2   | 69.5471   |
| 6                      | 1527.35  | 63.5739   |
| 7                      | 1490.7   | 67.915    |
| 8                      | 1429.96  | 65.582    |
| 9                      | 1334.5   | 70.5909   |
| 10                     | 1296.89  | 76.2428   |
| 11                     | 1232.29  | 68.5458   |
| 12                     | 1185.04  | 61.0644   |
| 13                     | 1126.22  | 54.2277   |
| 14                     | 1089.58  | 61.7776   |
| 15                     | 1040.41  | 49.2693   |
| 16                     | 909.272  | 81.0263   |
| 17                     | 830.205  | 62.9343   |
| 18                     | 725.104  | 82.2448   |



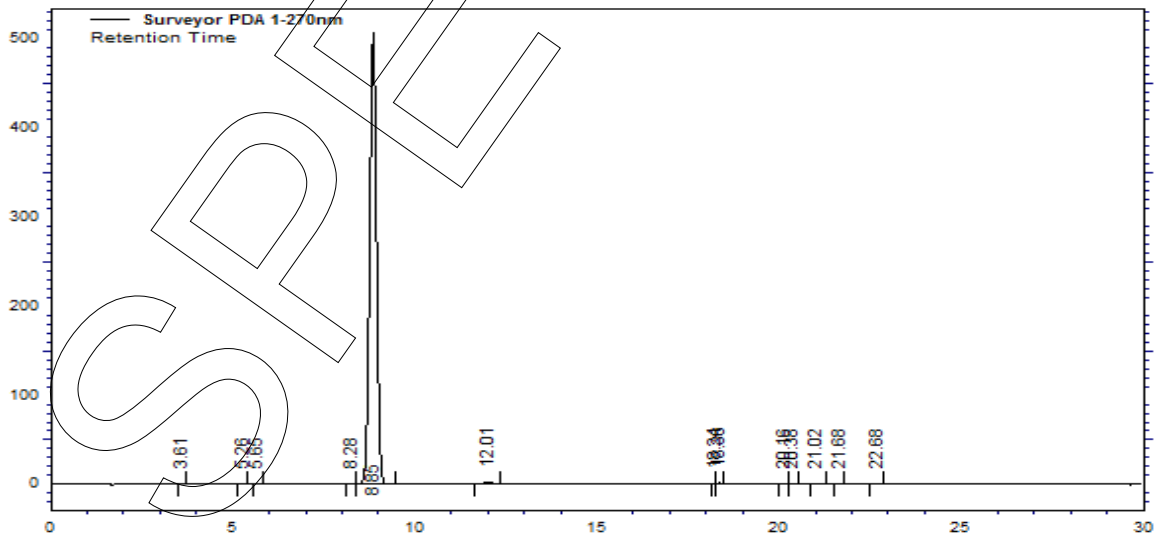
## Assay

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 µm, 150 x 4.6 mm  |
| Column temperature | 40 °C  |
| Detector           | DAD, 270 nm  |
| Injector           | Auto 5.00 µl; 0.105 mg/ml in Acetonitrile  |
| Flow rate          | 1.0 ml/min   |
| Phase A            | Water, 0.1 % H <sub>3</sub> PO <sub>4</sub>  |
| Phase B            | Acetonitrile, 0.1 % H <sub>3</sub> PO <sub>4</sub>   |
| Gradient program   | 0-11 min A/B 60/40<br>11-15 min A/B to 35/65<br>15-20 min A/B 35/65<br>20-25 min A/B to 60/40<br>25-30 min A/B 60/40 (v/v) |

HPLC chromatogram and peak table





## Area percent report - sorted by signal

| Pk #          | Retention time | Area           | Area %        |
|---------------|----------------|----------------|---------------|
| 1             | 3.61           | 1005           | 0.02          |
| 2             | 5.26           | 869            | 0.01          |
| 3             | 5.65           | 704            | 0.01          |
| 4             | 8.28           | 1907           | 0.03          |
| 5             | 8.85           | 6450539        | 99.02         |
| 6             | 12.01          | 42556          | 0.65          |
| 7             | 18.24          | 1212           | 0.02          |
| 8             | 18.36          | 4749           | 0.07          |
| 9             | 20.16          | 1624           | 0.02          |
| 10            | 20.38          | 1031           | 0.02          |
| 11            | 21.02          | 4649           | 0.07          |
| 12            | 21.68          | 518            | 0.01          |
| 13            | 22.68          | 2980           | 0.05          |
| <b>Totals</b> |                | <b>6514343</b> | <b>100.00</b> |

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 = 6)**

99.02 %; SD = 0.01 %

### Volatile content

#### Water content

**Method**

Karl Fischer titration

**Result (n = 3)**

0.07 %; SD = 0.01 %



## Residual solvents

|                       |                               |
|-----------------------|-------------------------------|
| <b>Method</b>         | <sup>1</sup> H-NMR            |
| <b>Result (n = 1)</b> | Sum: 0.16 %<br>0.16 % Ethanol |

## Final result

**Assay "as is": 98.79 %**

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       | 04 Sep 2019 | Release of the Certificate of Analysis - initial version |

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