



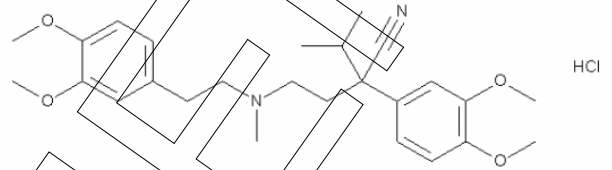
# Certificate of Analysis

ISO 9001

## Reference Material

### Product name

(2RS)-2-(3,4-Dimethoxyphenyl)-2-[2-[[2-(3,4-dimethoxy-phenyl)ethyl](methyl)amino]ethyl]-3-methyl-butanenitrile Hydrochloride



### Product code

MM0022.12-0025

### Lot number

1010628

### CAS number

1794-55-4

### Appearance

white solid

### Molecular weight

477.04

### Melting point

181 °C

### Molecular formula

C<sub>26</sub>H<sub>36</sub>N<sub>2</sub>O<sub>4</sub> HCl

### Long-term storage

2 to 8 °C, dark

Assay "as is"  
96.6 %

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

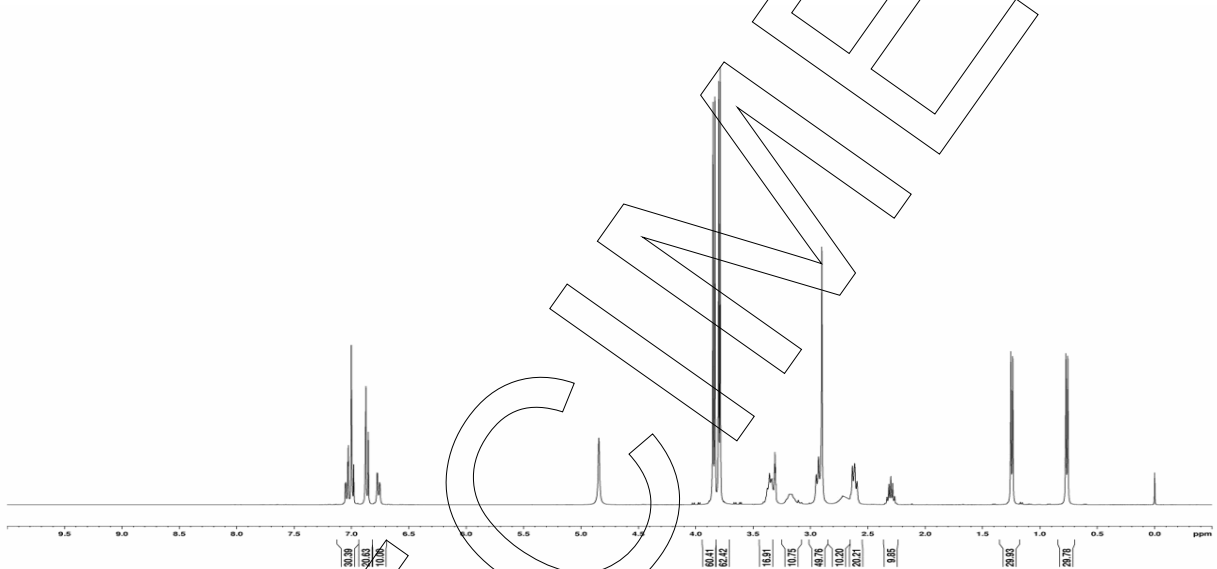
SPECIMEN



### Identity

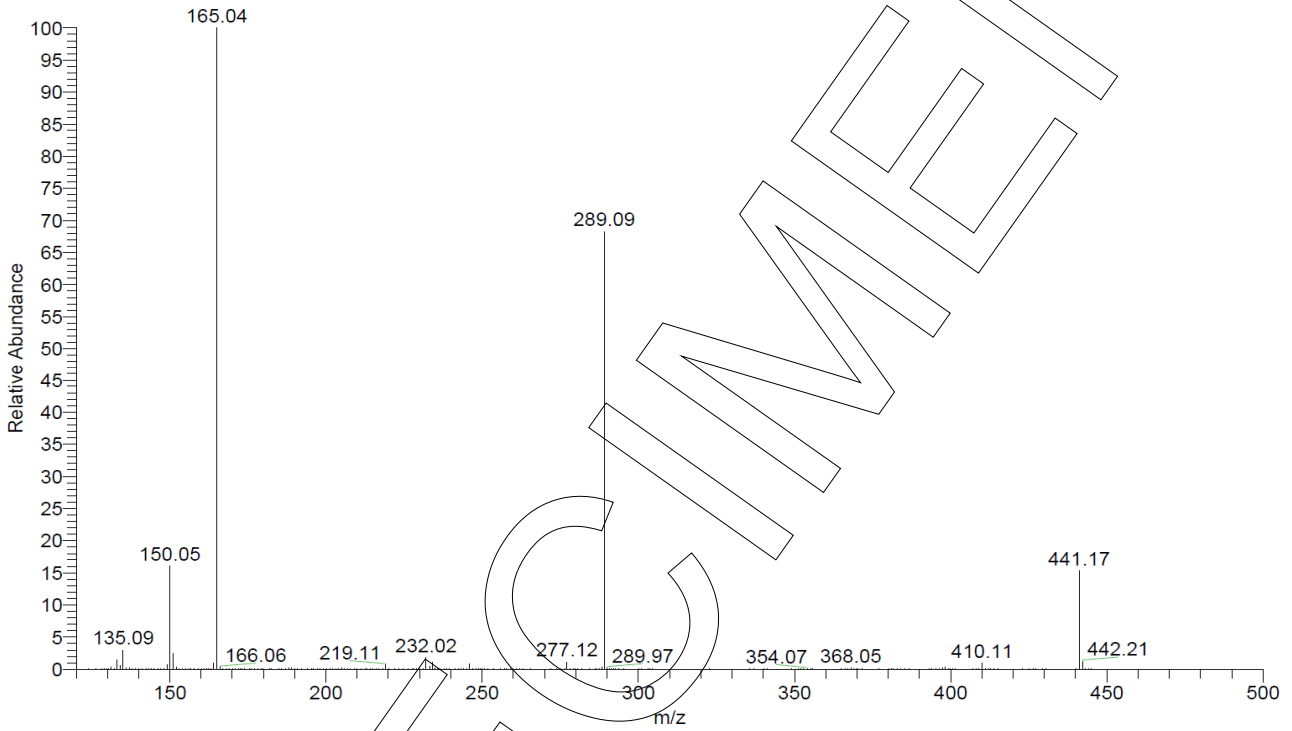
The identity of the reference material was established by following analyses.

Method	Conditions	Result
<sup>1</sup> H-NMR	400 MHz, CD <sub>3</sub> OD	Structure confirmed





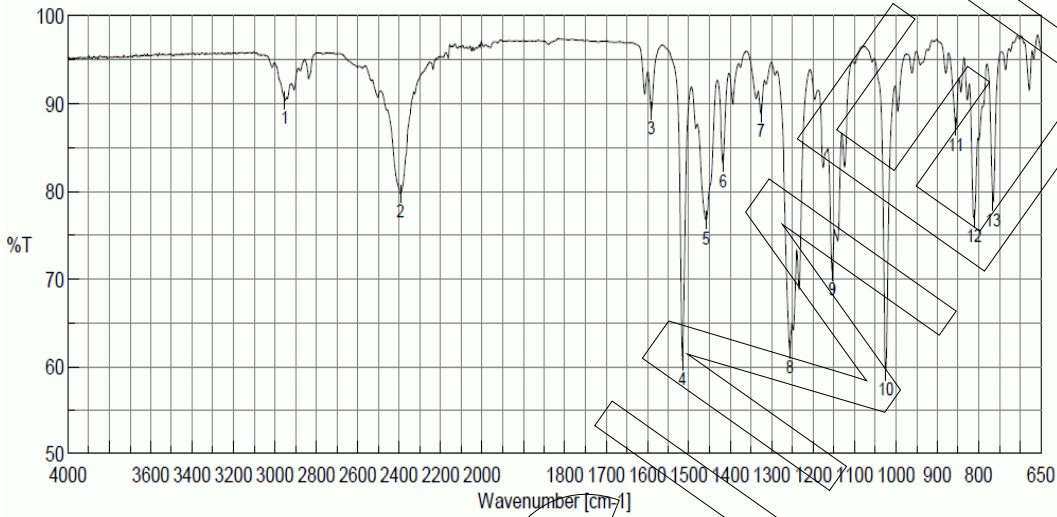
Method	Conditions	Result
MS	4.5 kV ESI+; vaporization temperature: 200 °C	Structure confirmed



SPRECHMANN



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



Result of Peak Picking		
No.	Position	Intensity
1	2951.52	90.3099
2	2393.23	79.6932
3	1590.99	89.158
4	1515.78	60.5285
5	1458.89	76.6393
6	1417.42	83.1415
7	1325.82	88.8358
8	1256.4	61.8964
9	1154.19	70.7674
10	1024.02	59.3736
11	855.275	87.294
12	810.92	76.8857
13	765.601	78.7176

SPECS



## Assay

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

### Purity by High Performance Liquid Chromatography (HPLC)

HPLC Conditions:	
Column	Ascentis Express C18; 2.7 µm, 150 x 4.6 mm
Column temperature	40 °C
Detector	DAD, 278 nm
Injector	Auto 5.00 µl; 0.402 mg/ml in Water/Acetonitrile 50/50 (v/v); 0.2 % Triethylamine
Flow rate	1.0 ml/min
Phase A	2 ml/l Triethylamine in Water
Phase B	2 ml/l Triethylamine in Acetonitrile
Gradient program	0-10 min A/B 50/50 10-15 min A/B to 30/70 15-20 min A/B to 50/50 20-30 min A/B 50/50 (v/v)

HPLC chromatogram and peak table





## Area percent report - sorted by signal

Pk #	Retention time	Area	Area %
1	1.06	1861	0.03
2	1.41	2617	0.04
3	1.55	8065	0.13
4	1.66	8108	0.13
5	1.77	1959	0.03
6	1.91	473	0.01
7	2.07	1805	0.03
8	2.26	1057	0.02
9	2.37	7928	0.13
10	2.74	474	0.01
11	2.89	835	0.01
12	3.29	1452	0.02
13	3.61	545	0.01
14	4.13	560	0.01
15	4.36	7835	0.12
16	4.65	3065	0.05
17	5.17	2934	0.05
18	6.17	922	0.01
19	6.77	1583	0.03
20	7.42	87877	1.39
21	7.91	6125158	96.91
22	8.63	3102	0.05
23	8.88	10163	0.16
24	9.14	2915	0.05



25	9.61	1190	0.02
26	10.84	1200	0.02
27	11.77	13943	0.22
28	12.88	8913	0.14
29	13.38	11746	0.19
<b>Totals</b>		<b>6320285</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.

<b>Result (n = 6)</b>	96.90 %; SD = 0.02 %
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## Volatile content

<b>Water content</b>	
<b>Method</b>	Karl Fischer titration
<b>Result (n = 3)</b>	0.33 %; SD = 0.01 %

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





## Final result

**Assay "as is": 96.58 %**

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.