



Certificate of Analysis

ISO 9001

Reference Material

Product name

7-(4-[4-[4-(2,3-Dichlorophenyl)piperazin-1-yl]butoxy]butoxy)-3,4-dihydroquinolin-2(1H)-one

Product code

MM0961.05-0025

CAS number

not listed

Molecular weight

520.49

Molecular formula

C₂₇H₃₅Cl₂N₃O₃

Lot number

1011826

Appearance

white solid

Melting point (DSC)

106 °C

Long-term storage

2 to 8 °C, dark



Assay "as is"
96.9 %

Date of shipment:

02 Sep 2019

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, 06 Aug 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

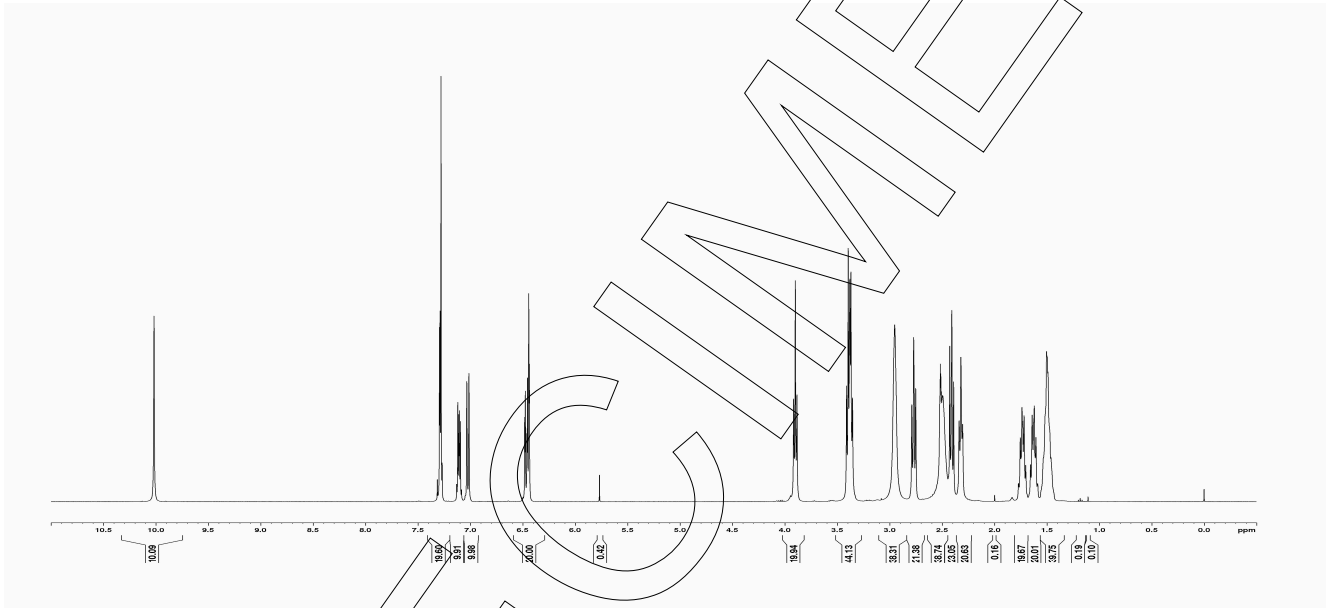
SPECIMEN



Identity

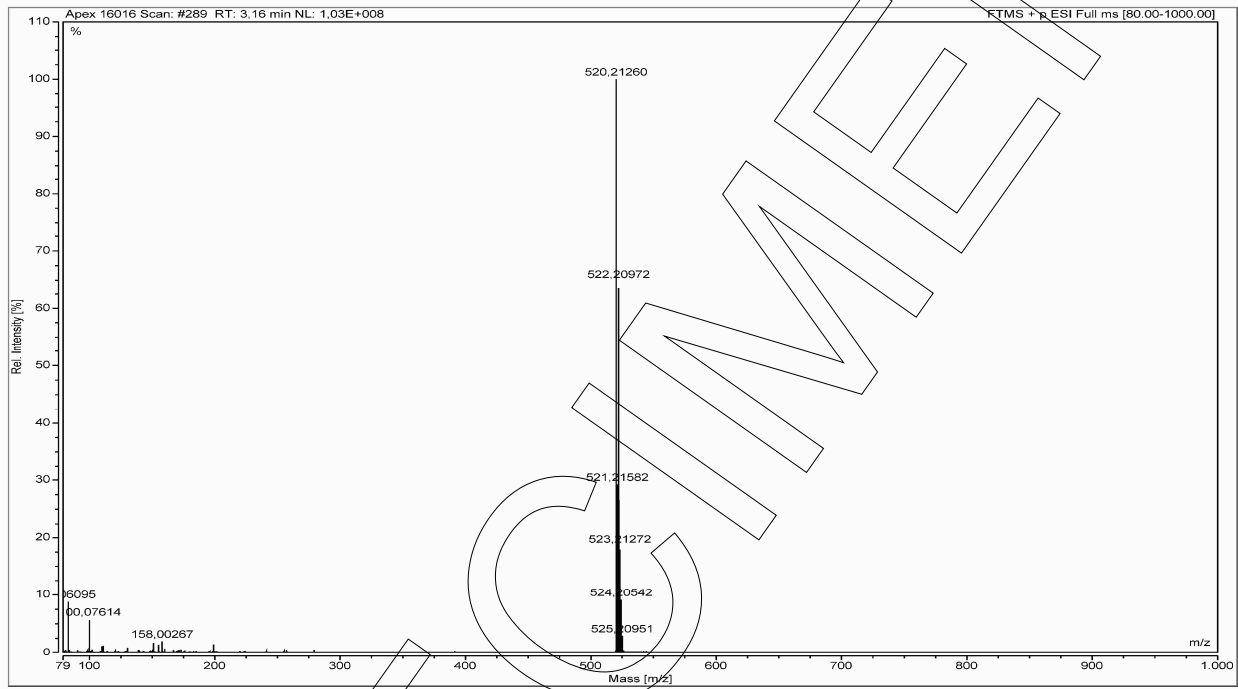
The identity of the reference material was established by following analyses.

Method	Conditions	Result
¹ H-NMR	400 MHz, DMSO-d ₆	Structure confirmed



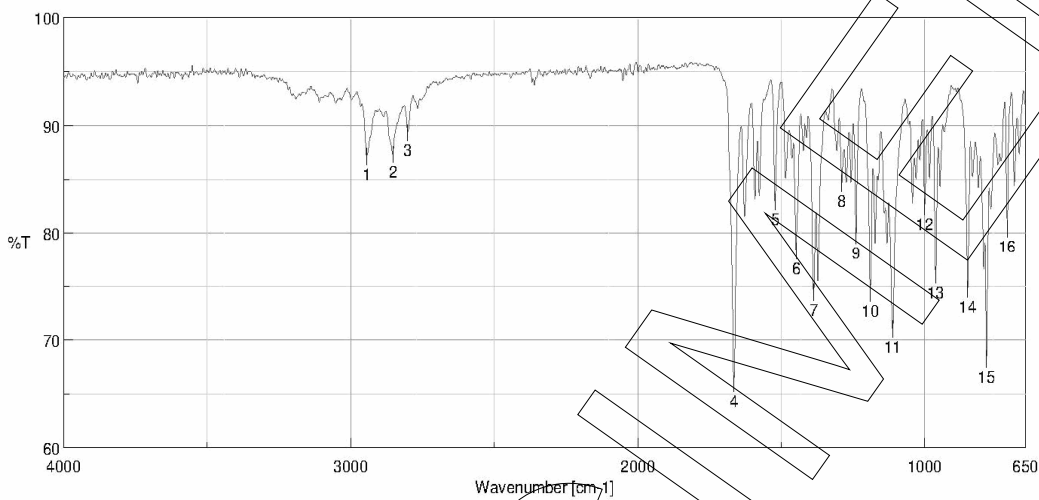


Method	Conditions	Result
MS	3.5 kV ESI+; capillary temperature: 269 °C Theoretical value: 520.21282	Structure confirmed





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



Results of Peak Find		
No.	Position	Intensity
1	2943.8	87.0973
2	2853.17	87.3431
3	2801.1	89.3573
4	1665.23	65.9983
5	1521.56	82.9423
6	1448.28	78.2438
7	1387.53	74.4007
8	1289.18	84.5942
9	1240	79.7561
10	1189.86	74.2972
11	1111.76	70.9686
12	999.91	82.4688
13	962.305	76.0661
14	850.454	74.7537
15	784.886	68.1871
16	712.569	80.3522

Assay

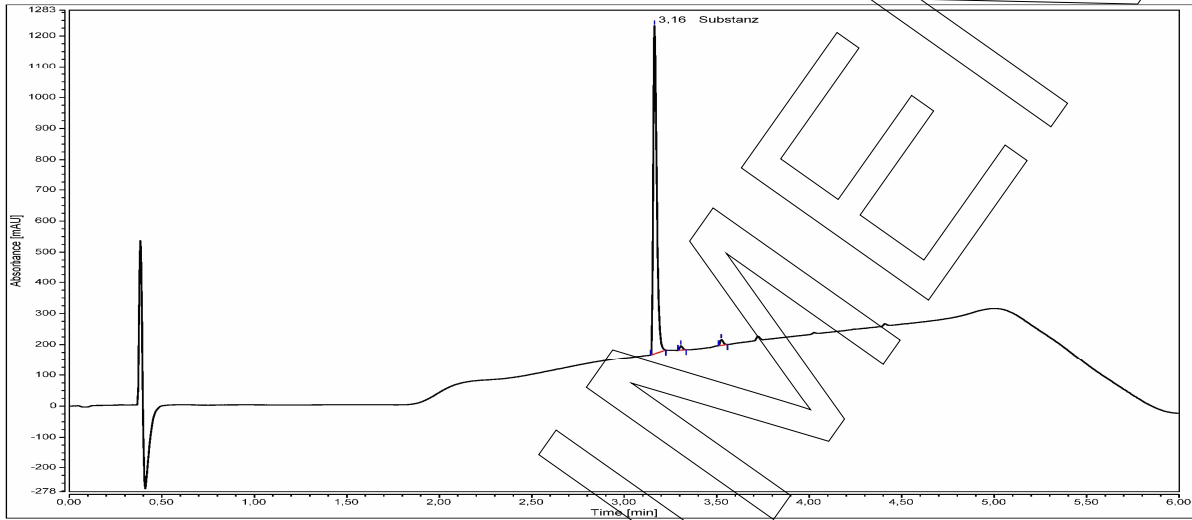
The assay of the reference material was assessed by following analyses.

Purity by High Performance Liquid Chromatography (HPLC)

HPLC Conditions:	
Column	Cortecs UPLC C18 +; 1.6 µm, 75 x 2.1 mm
Column temperature	40 °C
Detector	DAD, 220 nm
Injector	Auto 1 µl; 0.052 mg/ml in Acetonitrile
Flow rate	0.5 ml/min
Phase A	Water, 0.1 % HCOOH
Phase B	Acetonitrile, 0.1 % HCOOH
Gradient program	0-1 min A/B 98/2 1-4 min A/B to 2/98 4-5 min A/B to 98/2 5-6 min A/B 98/2 (v/v)



HPLC chromatogram and peak table



Area percent report - sorted by signal

Pk #	Retention time	Area	Area %	
1	3.163	23.5385	97.44	
2	3.306	0.2503	1.04	
3	3.525	0.3681	1.52	
Totals		24.1569	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)

97.44 %; SD < 0.01 %



Volatile content

Water content

Method	Karl Fischer titration
Result (n = 3)	0.11 %; SD = 0.01 %

Residual solvents

Method	¹ H-NMR
Result (n = 1)	Sum: 0.46 % 0.09 % Ethyl acetate; 0.35 % Methylene chloride 0.02 % Methyl tert-butyl ether

Final result

Assay "as is": 96.88 %

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	06 Aug 2019	Release of the Certificate of Analysis - initial version

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