

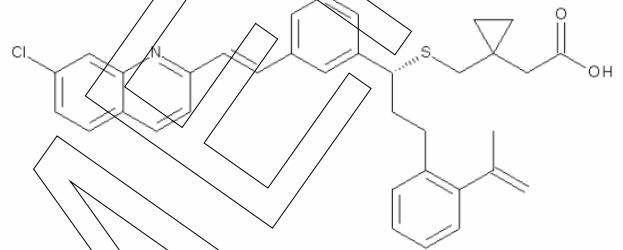
Certificate of Analysis

ISO 9001

Reference Material

Product name

[1-[[[(1R)-1-[3-[(E)-2-(7-Chloroquinolin-2-yl)ethenyl]phenyl]-3-[2-(1-methylethenyl)phenyl]propyl]sulfanyl]methyl]cyclopropyl]acetic Acid



Product code

MM0698.02

Lot number

1013054

CAS number

918972-54-0

Appearance

yellow solid

Molecular weight

568.17

Melting point (DSC)

162 °C

Molecular formula

C₃₅H₃₄ClNO₂S

Long-term storage

2 to 8 °C, dark

Assay "as is"
97.0 %

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

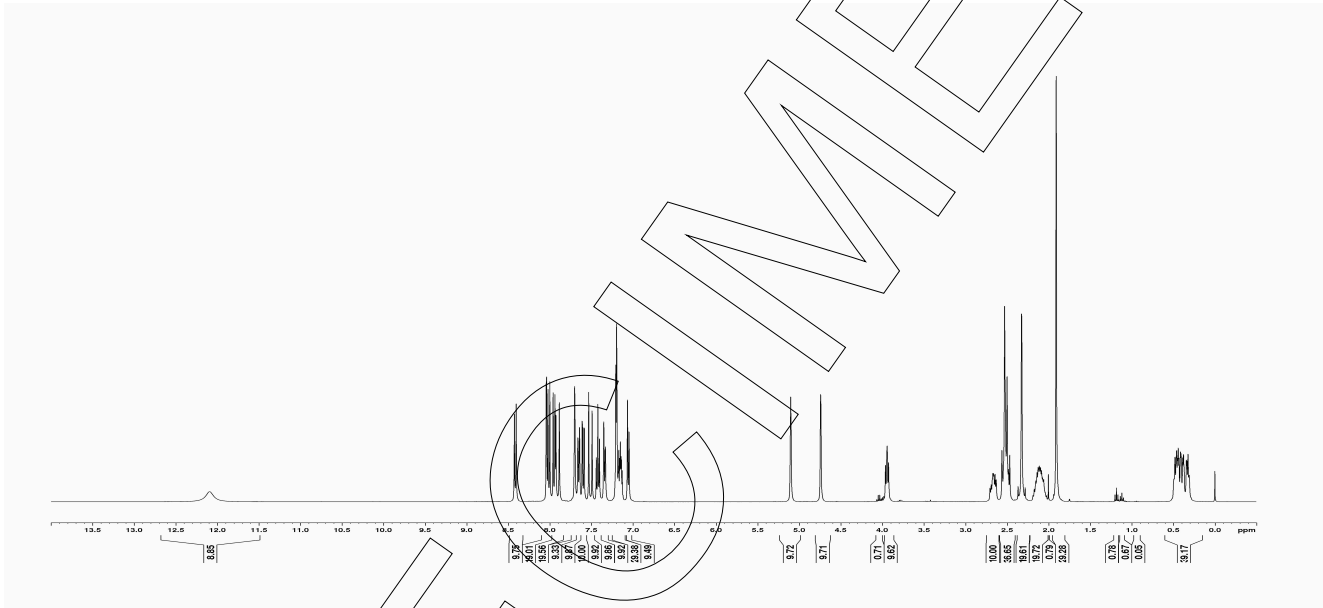
SPECIMEN



Identity

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

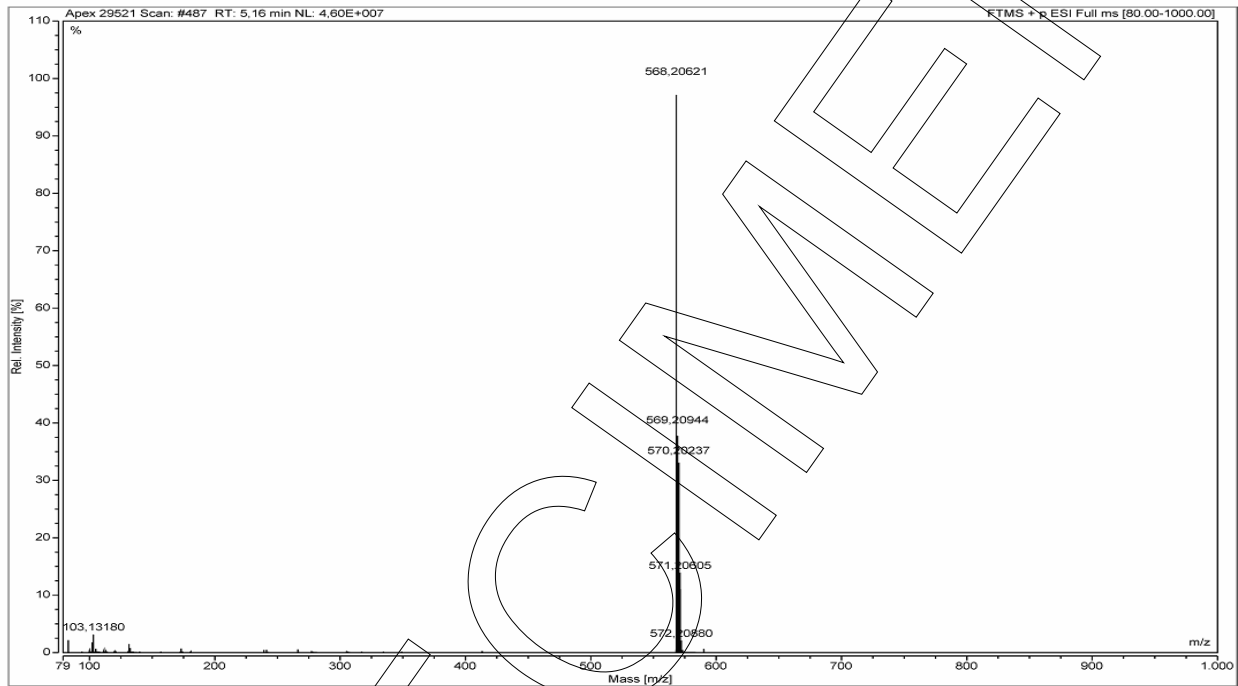
Method	Conditions	Result
¹ H-NMR	400 MHz, DMSO-d ₆	Structure confirmed



SAMPLE

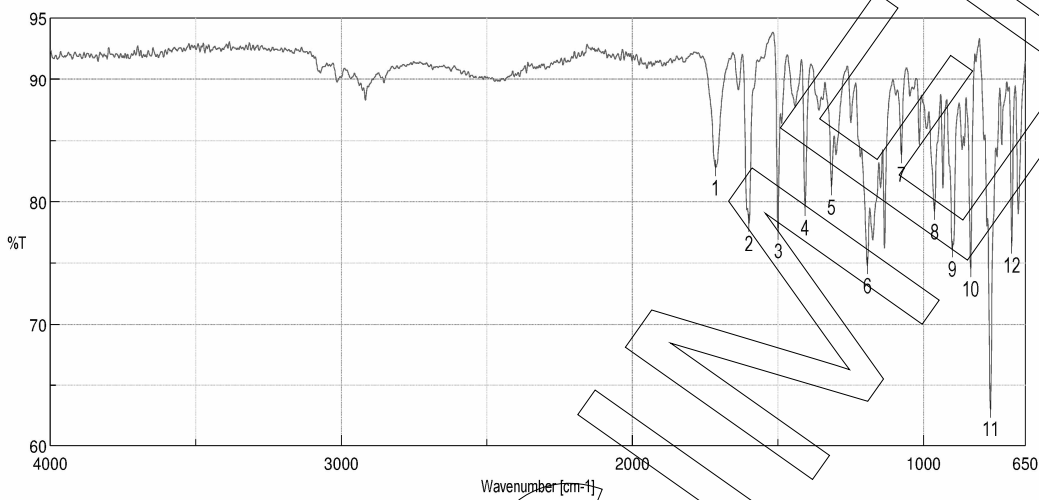


Method	Conditions	Result
MS	3.5 kV ESI+; capillary temperature: 269 °C Theoretical value: 568.20715	Structure confirmed





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



No.	Position	Intensity
1	1713.44	82.7143
2	1599.66	78.2655
3	1499.38	77.6356
4	1406.82	79.5234
5	1316.18	81.1912
6	1192.76	74.7595
7	1076.08	83.8444
8	962.305	79.2124
9	901.558	76.1192
10	837.919	74.5399
11	769.458	63.0362
12	696.177	76.4285

Assay

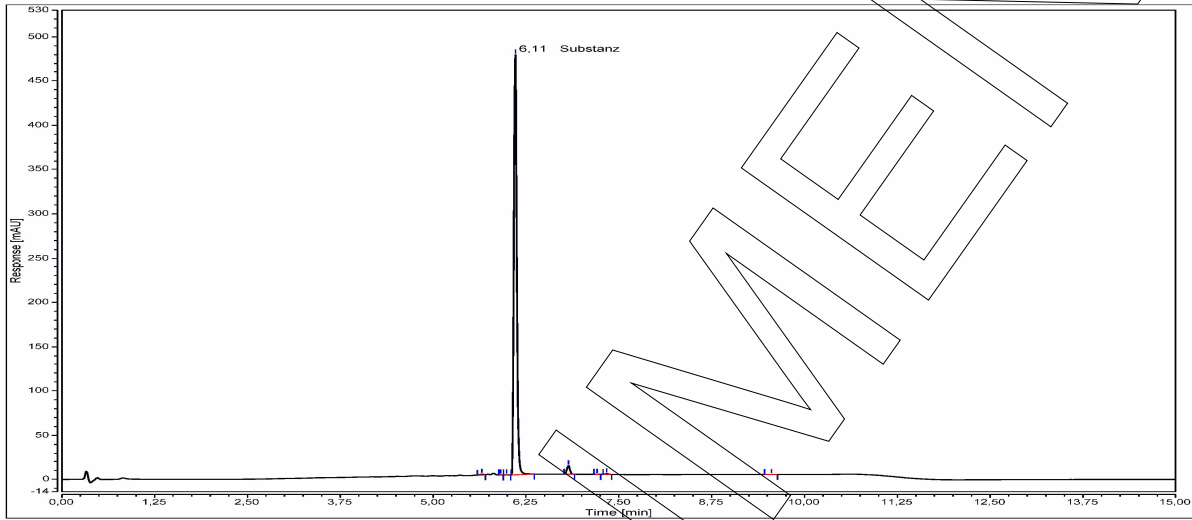
The assay of the reference material was assessed by following analyses.

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, 210 nm
Injector	Auto 3 µl; 0.052 mg/ml in Methanol
Flow rate	0.5 ml/min
Phase A	Water
Phase B	Acetonitrile
Gradient program	0-1 min A/B 98/2 1-4 min A/B to 2/98 4-9 min A/B 2/98 9-10 min A/B to 98/2 10-15 min A/B 98/2 (v/v)



HPLC chromatogram and peak table



SPECIMEN



Area percent report - sorted by signal

Pk #	Retention time	Area	Area %
1	5.656	0.0559	0.24
2	5.910	0.0030	0.01
3	5.990	0.0099	0.04
4	6.110	22.2888	97.52
5	6.823	0.4446	1.95
6	7.210	0.0082	0.04
7	7.336	0.0410	0.18
8	9.556	0.0048	0.02
Totals		22.8562	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)

97.52 %; SD = 0.01 %

Volatile content

Water content

Method

Karl Fischer titration

Result

No significant amounts of water were detected (< 0.05 %).

Residual solvents

Method

¹H-NMR

Result (n = 1)

Sum: 0.55 %

0.14 % Diethyl ether; 0.40 % Ethyl acetate
0.01 % Triethylamine



Final result

Assay "as is": 96.98 %

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.