



Certificate of Analysis

ISO 9001

Reference Material

Product name

11,11'-[Ethylenebis(oxyethylenepiperazine-4,1-diyl)]bis(dibenzo[b,f][1,4]thiazepine) Tetrahydrochloride

Product code

MM1130.25-0025

CAS number

1923194-81-3

Molecular weight

850.79

Molecular formula

C₄₀H₄₄N₆O₂S₂ 4HCl

Lot number

1011783

Appearance

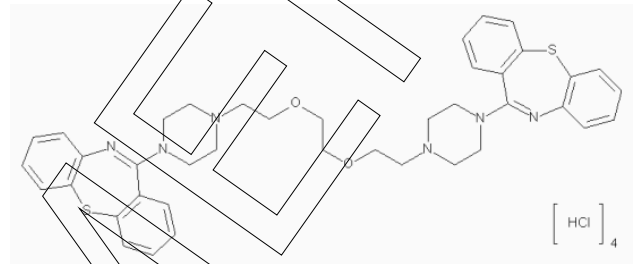
white solid

Melting point

219 °C (dec)

Long-term storage

2 to 8 °C, dark



Assay "as is"
90.8 %

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

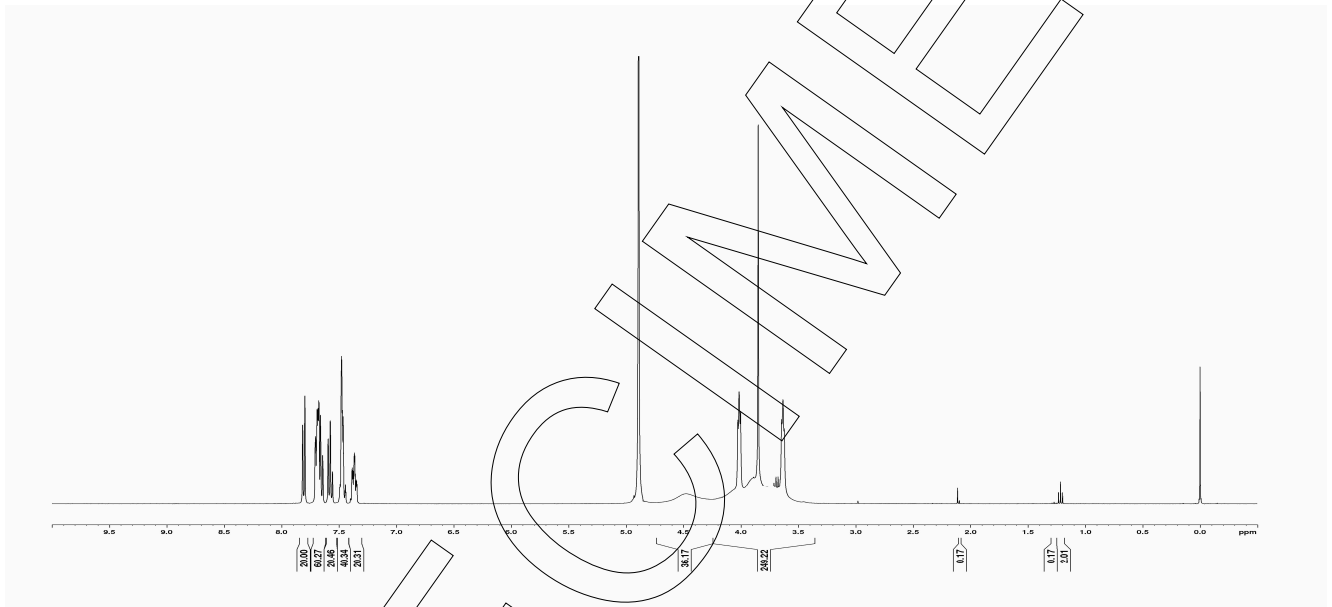
SPECIMEN



Identity

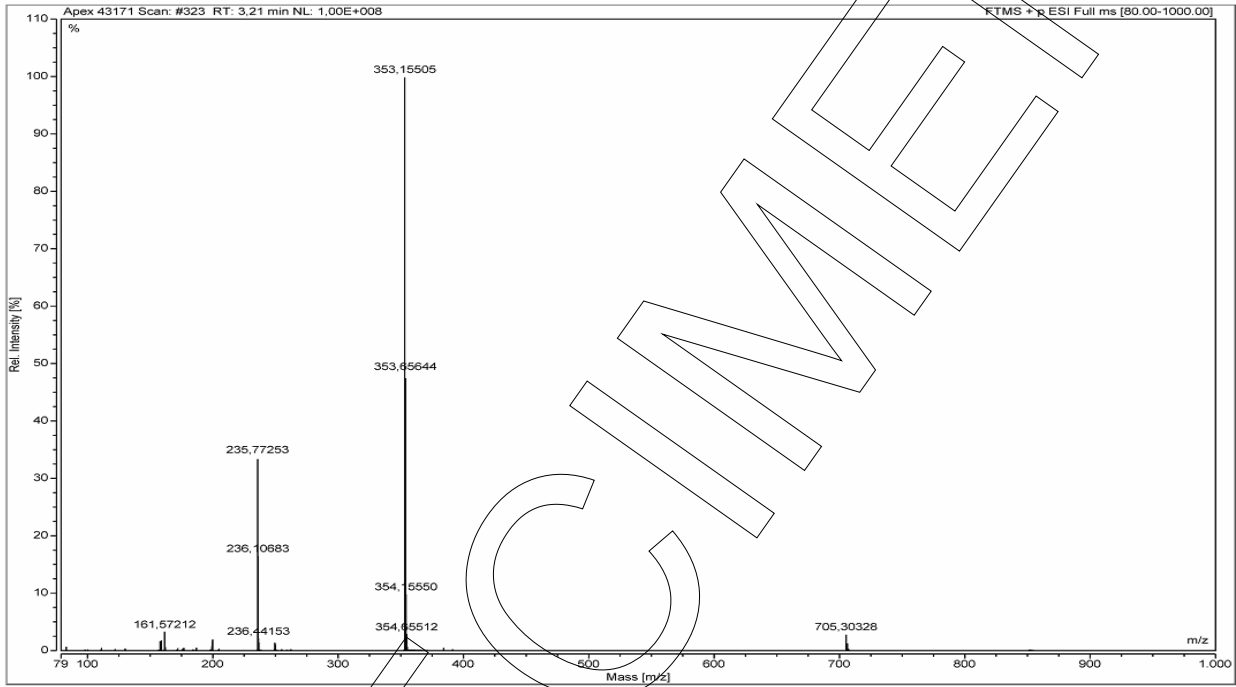
The identity of the reference material was established by following analyses.

Method	Conditions	Result
¹ H-NMR	400 MHz, D ₂ O	Structure confirmed





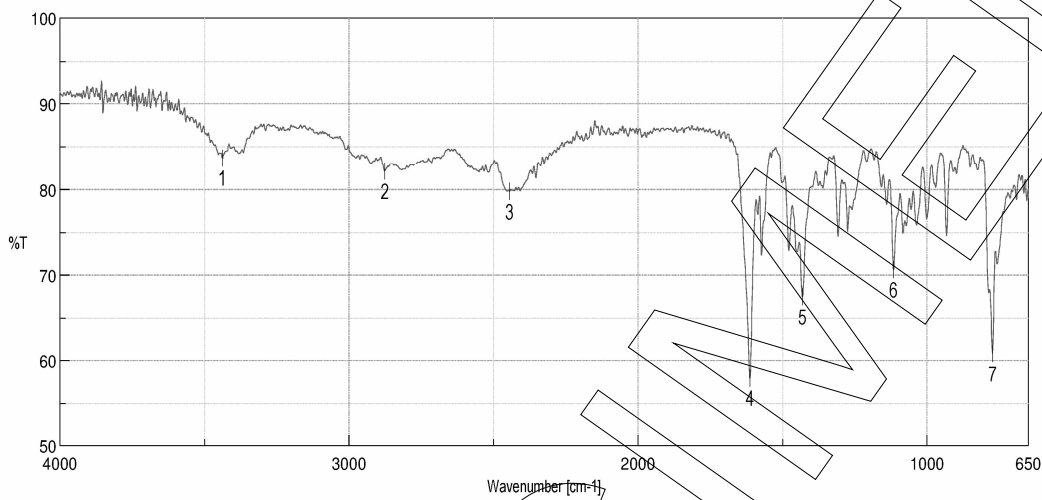
Method	Conditions	Result
MS	3.5 kV ESI+; capillary temperature: 269 °C Theoretical value: 705.30399	Structure confirmed



SAMPLE



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



Results of Peak Find		
No.	Position	Intensity
1	3438.46	83.6351
2	2876.31	82.08
3	2444.33	79.724
4	1613.16	57.9033
5	1431.89	67.5007
6	1116.58	70.5851
7	774.279	60.7859

Assay

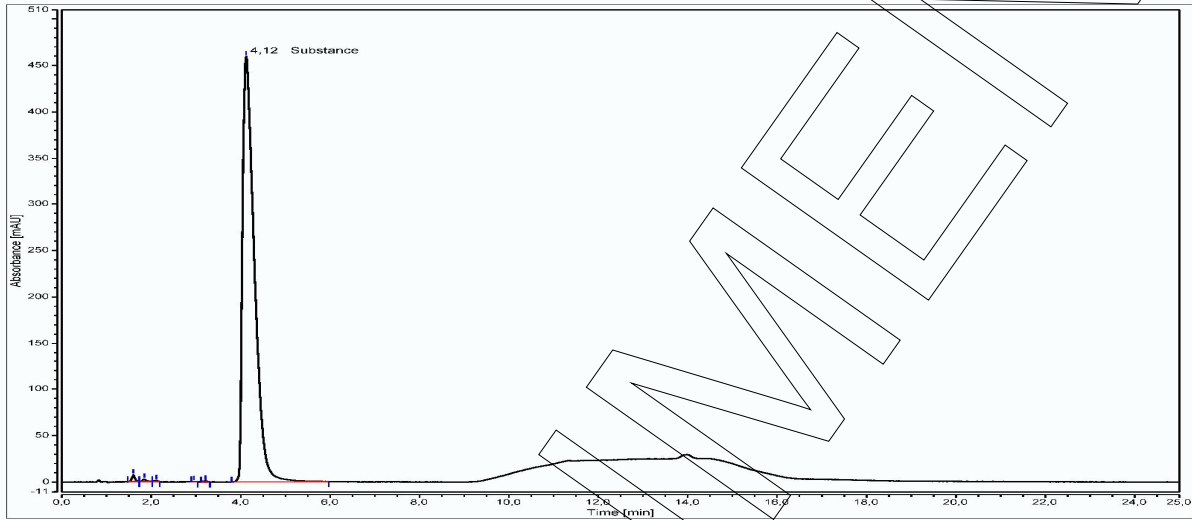
The assay of the reference material was assessed by following analyses.

Purity by High Performance Liquid Chromatography (HPLC)

HPLC Conditions:	
Column	LiChrospher 60 RP-select B; 5 µm, 125 x 4.0 mm
Column temperature	40 °C
Detector	DAD, 210 nm
Injector	Auto 5 µl; 0.102 mg/ml in Acetonitrile/Water 50/50 (v/v)
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	0-7 min A/B 55/45 7-9 min A/B to 20/80 9-12 min A/B 20/80 12-14 min A/B to 55/45 14-25 min A/B 55/45 (v/v)



HPLC chromatogram and peak table



Area percent report - sorted by signal

Pk #	Retention time	Area	Area %
1	1.597	0.5978	0.42
2	1.843	0.2930	0.21
3	2.113	0.1321	0.09
4	2.953	0.0364	0.03
5	3.217	0.1193	0.08
6	4.123	140.5673	99.17
Totals		141.7459	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)

99.15 %; SD = 0.03 %

Volatile content

Water content

Method

Karl Fischer titration

Result (n = 3)

8.05 %; SD = 0.06 %

Residual solvents

Method

¹H-NMR

Result (n = 1)

Sum: 0.42 %

0.36 % Ethanol; 0.06 % Ethyl acetate

Final result

Assay "as is": 90.75 %

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.

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