



Certificate of Analysis

ISO 9001

Reference Material

Product name

Methyl (1,1-Dioxido-3-oxo-1,2-benzisothiazol-2(3H)-yl)acetate

Product code

MM0084.07-0025

CAS number

6639-62-9

Molecular weight

255.25

Molecular formula

C₁₀H₉NO₅S

Lot number

1191246

Appearance

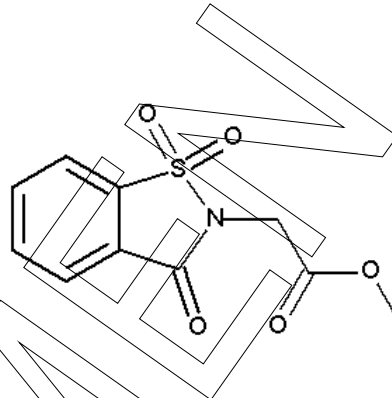
white solid

Melting point

120 °C

Long-term storage

2 to 8 °C, dark



Assay "as is"
99.6 %

Date of shipment:

08 Nov 2021

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.

Release by:	Date of Release:		Product Release
Dr. Sabine Schröder	Luckenwalde, 04 Nov 2021		



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

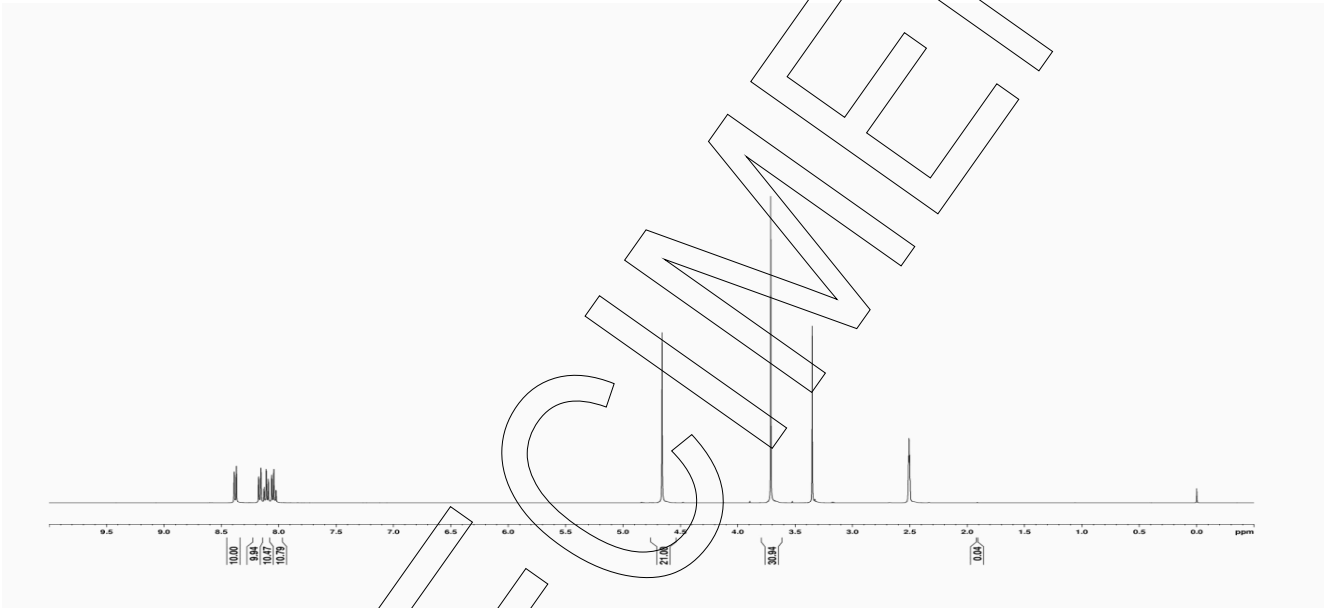
SPECIMEN



Identity

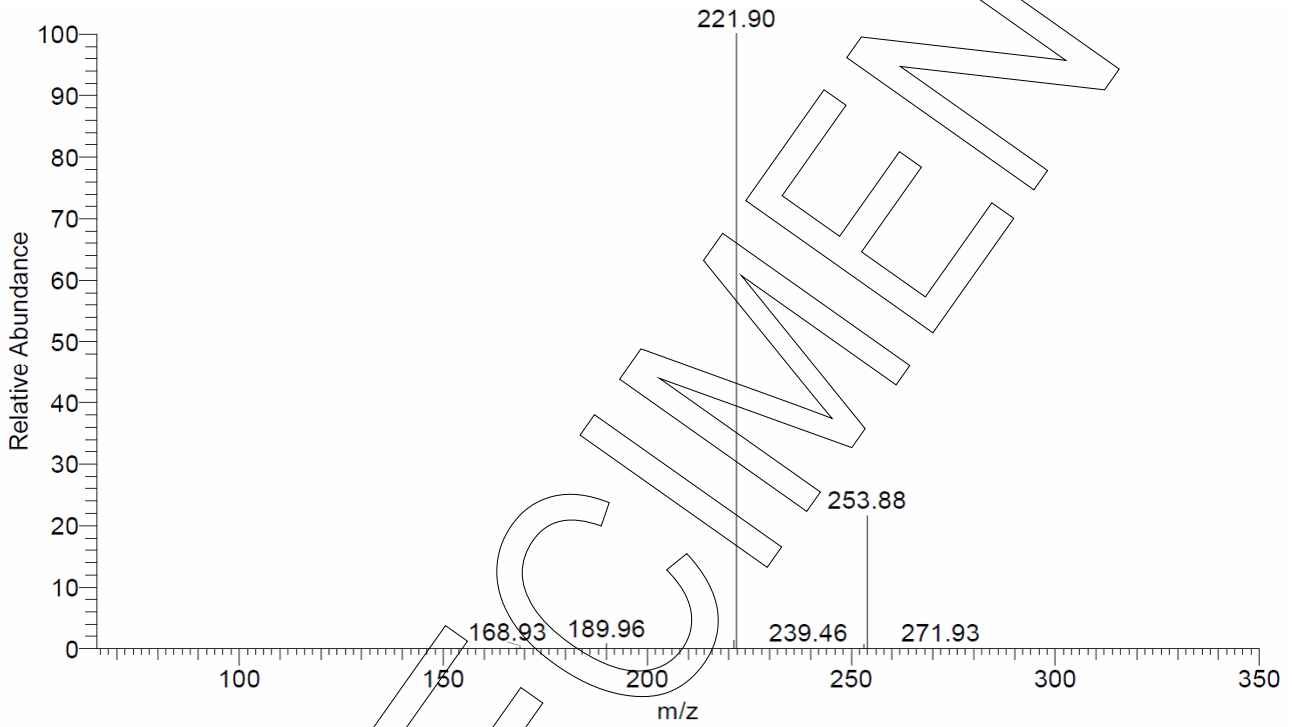
The identity of the reference material was established by following analyses.

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



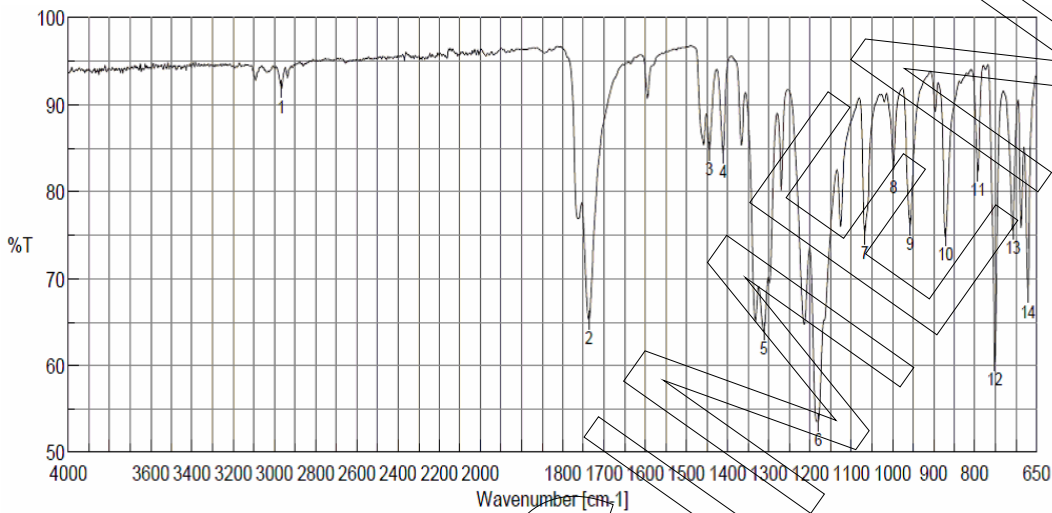


Method	Conditions	Result
MS	4.5 kV ESI-; vaporization temperature: 200 °C	Structure confirmed





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



No.	Position	Intensity
1	2965.98	91.7293
2	1736.58	65.1417
3	1444.42	84.5954
4	1410.67	84.2555
5	1312.32	63.9161
6	1180.22	53.3859
7	1067.41	74.9808
8	997.982	82.5026
9	956.52	75.9542
10	870.703	74.7578
11	792.6	82.2576
12	751.138	60.3691
13	707.747	75.524
14	671.106	68.1885

Assay

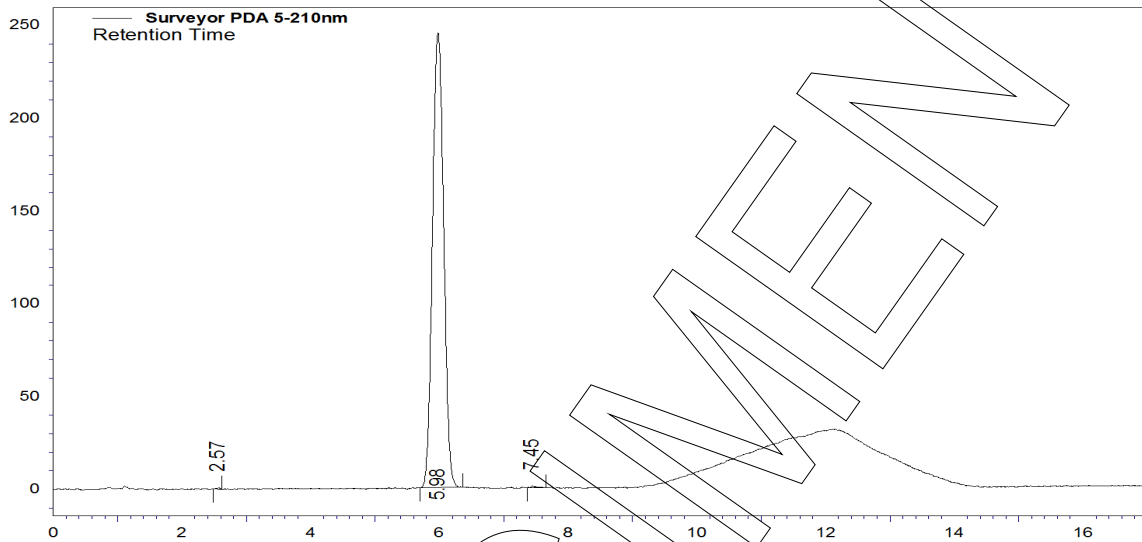
The assay of the reference material was assessed by following analyses.

Purity by High Performance Liquid Chromatography (HPLC)

HPLC Conditions:	
Column	Purospher RP-18e; 5 µm, 125 x 4.0 mm
Column temperature	40 °C
Detector	DAD, 210 nm
Injector	Auto 4 µl; 0.051 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 75/25 7-10 min A/B to 30/70 10-12 min A/B to 75/25 12-17 min A/B 75/25 (v/v)



HPLC chromatogram and peak table



Area percent report - sorted by signal

Pk #	Retention time	Area	Area %
1	2.57	3030	0.10
2	5.98	2974156	99.67
3	7.45	6959	0.23
Totals		2984145	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)

99.66 %; SD = 0.05 %



Volatile content

Water content	
Method	Karl Fischer titration
Result (n = 3)	0.07 %; SD = 0.02 %

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

Final result

Assay "as is": 99.59 %

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 Nov 2021	Release of the Certificate of Analysis - initial version

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