



Mikromol™



Certificate of Analysis

ISO 9001

Reference Material

Product name

3-(2-Chlorophenyl)-5-methylisoxazole-4-carboxylic Acid

Product code

MM0682.04

CAS number

23598-72-3

Molecular weight

237.64

Molecular formula

C₁₁H₈ClNO₃

Lot number

1025256

Appearance

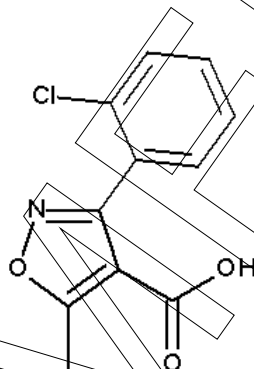
beige solid

Melting point

190 °C (dec)

Long-term storage

-18 °C, dark



Assay "as is"
99.2 %

Date of shipment:

02 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.

Release by:	Date of Release:		Product Release
Dr. Sabine Schröder	Luckenwalde, 01 Aug 2019		



MikromolTM

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

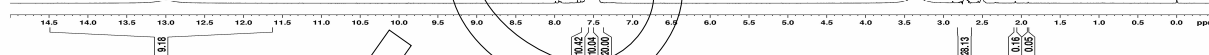
SPECIMEN



Identity

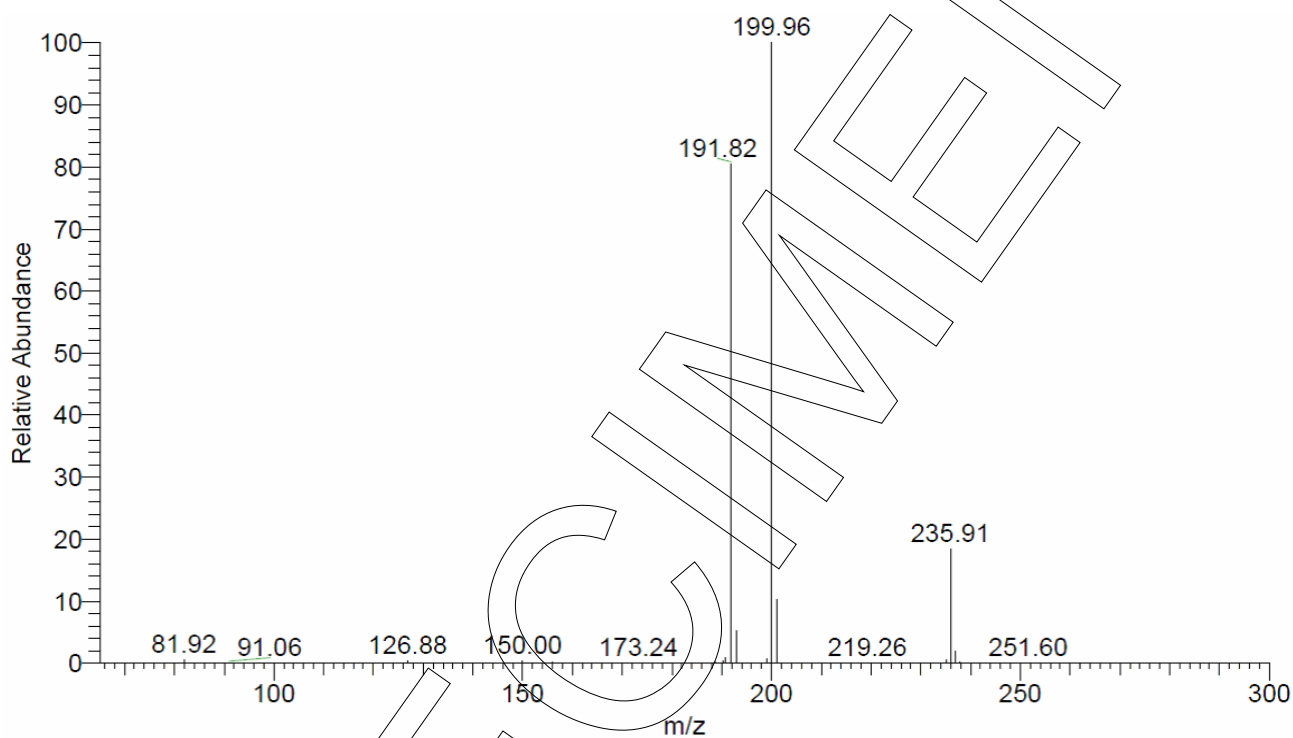
The identity of the reference material was established by following analyses.

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



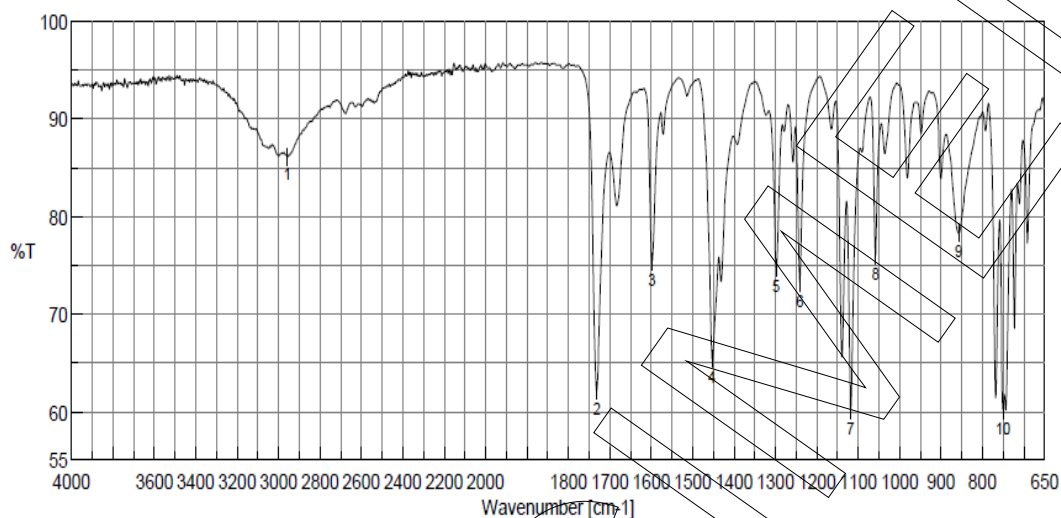


Method	Conditions	Result
MS	4.5 kV ESI; vaporization temperature: 200 °C	Structure confirmed





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



Result of Peak Picking		
No.	Position	Intensity
1	2956.34	86.0968
2	1731.76	62.0957
3	1597.73	75.3428
4	1452.14	65.3856
5	1297.86	74.7349
6	1240.97	73.0886
7	1117.55	60.1363
8	1058.73	75.9585
9	857.204	78.2322
10	750.174	60.1428

Assay

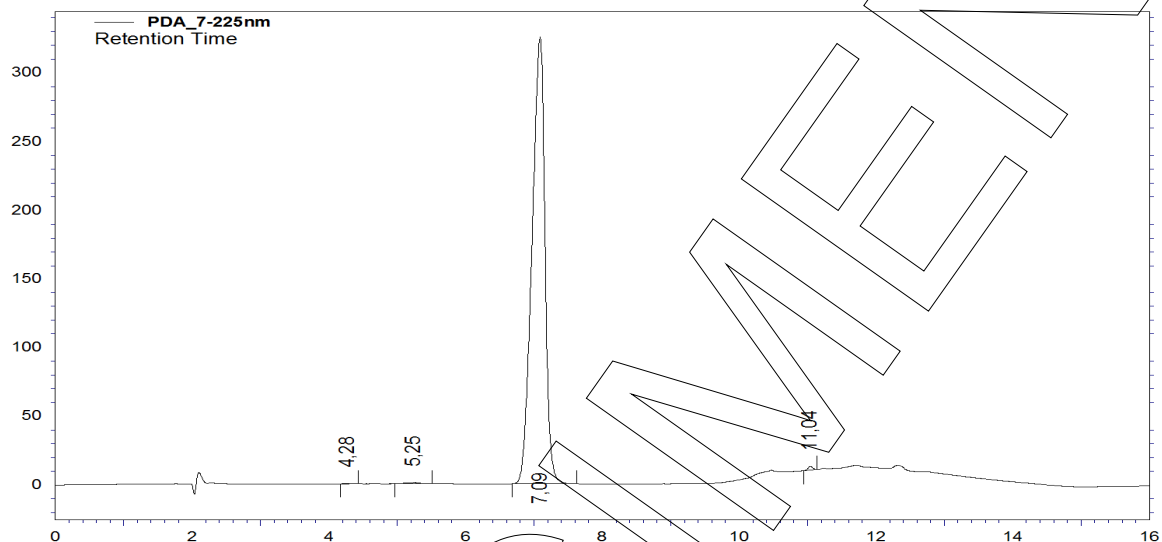
The assay of the reference material was assessed by following analyses.

Purity by High Performance Liquid Chromatography (HPLC)

HPLC Conditions:	
Column	Hypersil Gold C18; 5 µm, 150 x 4.6 mm
Column temperature	40 °C
Detector	DAD, 225 nm
Injector	Auto 5 µl; 0.092 mg/ml in Acetonitrile
Flow rate	1.0 ml/min
Phase A	2.7 g/l KH ₂ PO ₄ , pH 5.0
Phase B	Acetonitrile
Gradient program	0-6 min A/B 85/15 6-9 min A/B to 50/50 9-11 min A/B to 85/15 11-16 min A/B 85/15 (v/v)



HPLC chromatogram and peak table



Area percent report - sorted by signal

Pk #	Retention time	Area	Area %	
1	4.28	1687	0.04	
2	5.25	12078	0.28	
3	7.09	4273690	99.39	
4	11.04	12338	0.29	
Totals		4299793	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)

99.39 %; 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: 0.12 % 0.05 % Acetic acid; 0.07 % Acetone

Final result

Assay "as is": 99.16 %

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	01 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.