



Mikromol™



Certificate of Analysis

Characterisation methods are accredited according to

ISO 17025

Reference Material

Product name

(S)-2-Aminobutanamide Hydrochloride

Product code

MM1372.05-0025

CAS number

7682-20-4

Molecular weight

138.60

Molecular formula

C₄H₁₀N₂O · HCl

Lot number

W988173

Appearance

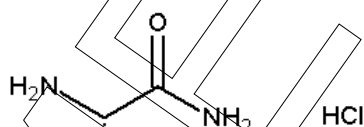
white solid

Melting point

258 °C (dec)

Long-term storage

2 to 8 °C, dark



Assay¹ "as is"
99.96 %

Uncertainty² U
0.4 %

Intended Use: Use for identification and quantification. The assay is verified by a second testing method.

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, 30 Jul 2019		

¹ Calibration and verification were carried out using standards traceable to SI-units. The value is expressed on an "as is" basis.

² The uncertainty "U" is the expanded uncertainty of the testing method for the assigned value estimated in accordance with the Guide to the Expression of Uncertainty in Measurement (GUM). It corresponds to a level of confidence of about 95%. Coverage factor k=2.



Product information

This RM is intended for laboratory use only and is not suitable for human or animal consumption.

This RM conforms to the characteristics of a primary standard as described in the ICH Guidelines. The values quoted in this Certificate of Analysis are the producer's best estimate of the true values within the stated uncertainties and based on the techniques described in this Certificate of Analysis. The characterisation of this material was undertaken in accordance with the requirements of ISO/IEC 17025. The identity is verified by data from international scientific literature.

Storage and handling

Before usage of the RM, it should be allowed to warm to room temperature. No drying is required, as assigned values are already corrected for the content of water and other volatile materials.

Reference Material quality is controlled by regularly performed quality control tests (retests).

Further content

Assigned value

Purity

Identity

Revision table



Assigned value

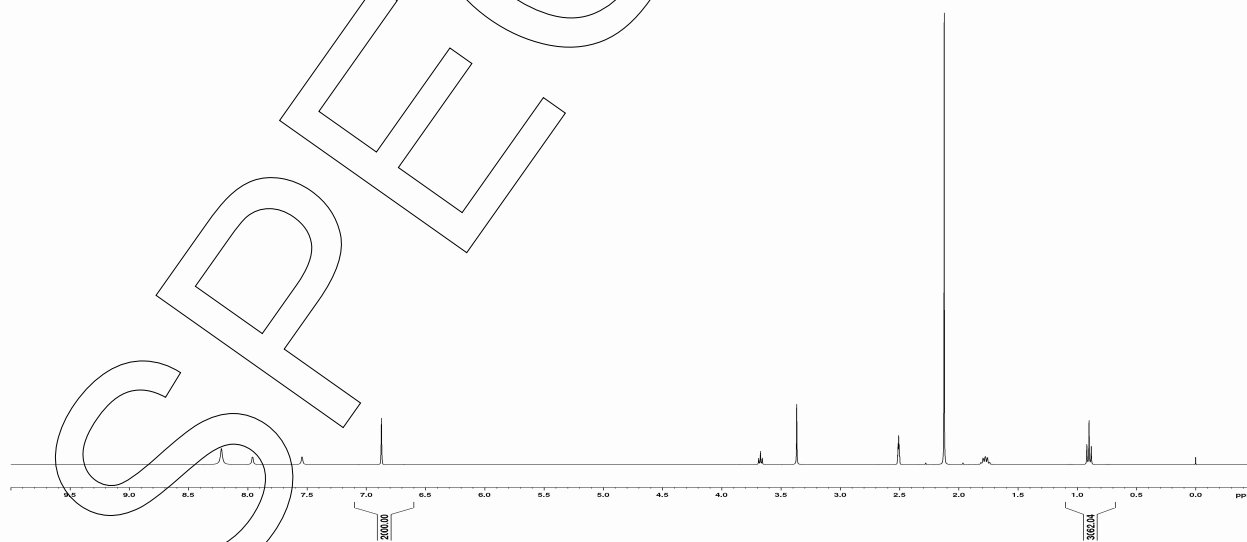
Assay "as is": 99.96 %; U = 0.42 %

The assay "as is" is assessed by quantitative NMR spectroscopy and is equivalent to the assay based on the not-anhydrous and not-dried substance. The assay is verified by elementary analysis (carbon titration). The verified result lies inside our acceptance criteria, i.e. less than 1.0 % difference to assay assigning technique.

For quantitative applications, use the assay as a calculation value on the "as is basis". The uncertainty of the assay can be used for estimation/calculation of measurement uncertainty.

Method 1: Value assigning technique - quantitative NMR spectroscopy	
Conditions	400 MHz, DMSO-d ₆
Internal standard	1,2,4,5-Tetramethylbenzene (certified reference material), signal 6.6 - 7.1 ppm, 2 H
Results (mass fraction, n = 6)	99.96 %; U = 0.42 %

Quantitative NMR spectrum





Method 2: Value verifying technique - carbon titration of elemental analysis

Method	percentage carbon found in relation to percentage carbon as calculated for molecular formula
Results (mass fraction, n = 3)	100.35 %

Volatile content

Water content

Method	Karl Fischer titration
Result (n = 3)	0.06 %*; SD = 0.01 %

*not accredited testing method

Residual solvents

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

*not accredited testing method

Inorganic residues

Method: Elementary analysis

Inorganic residues can be excluded by elementary analysis (CHN).



Mikromol™

Identity

The identity is assessed by ISO/IEC 17025 accredited testing methods.

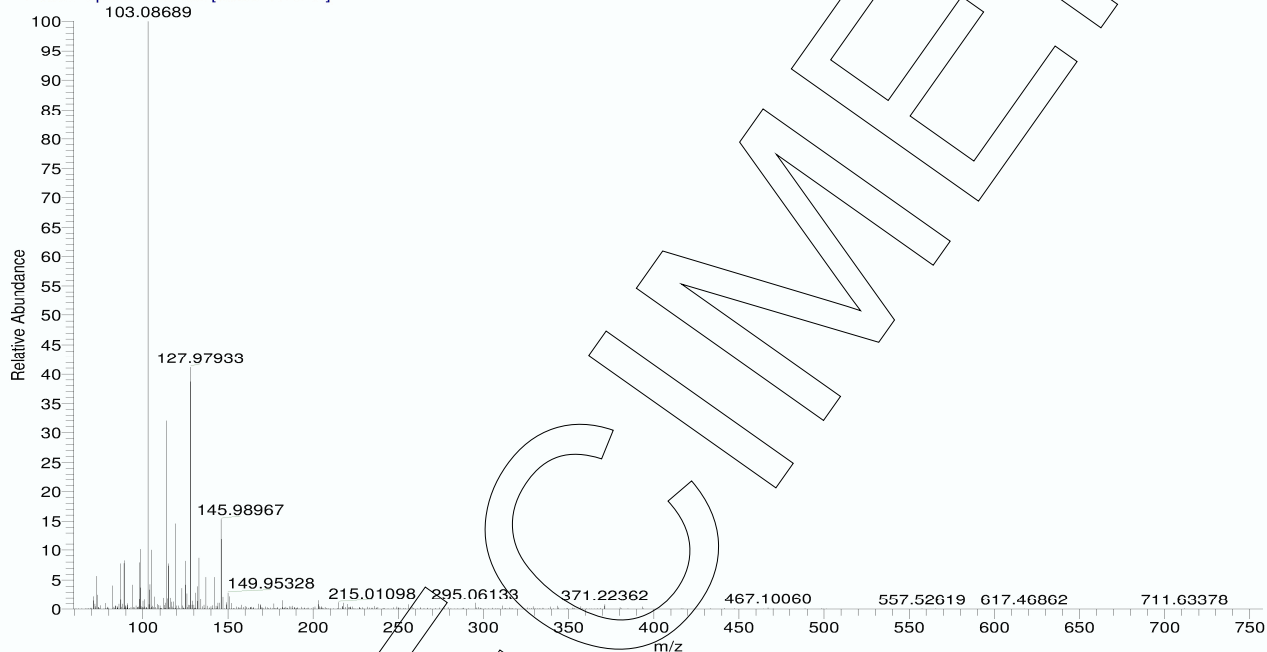
Method	Conditions	Result
¹ H-NMR	400 MHz, DMSO-d ₆	Structure confirmed





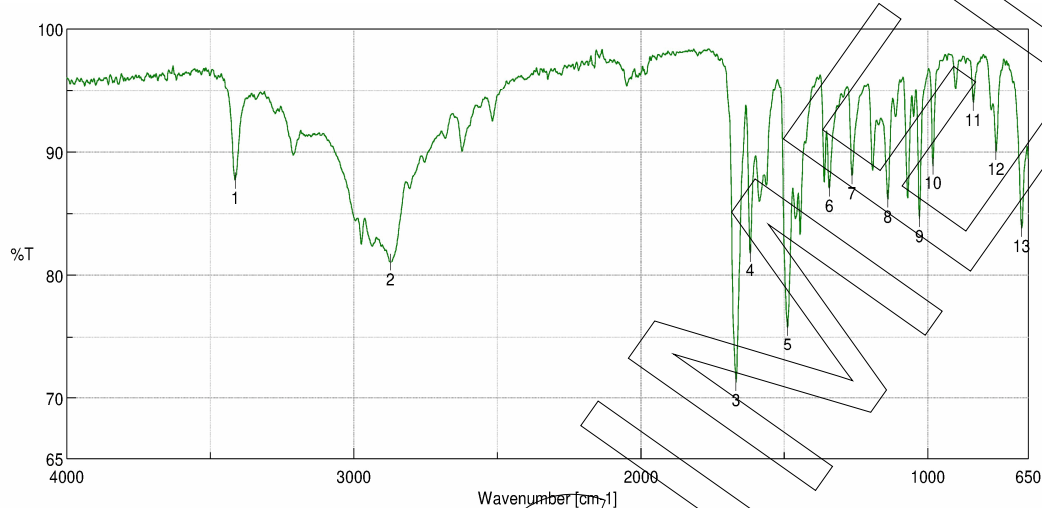
Method	Conditions	Result
MS	3 kV ESI+; capillary temperature: 269 °C Theoretical value: 103.08659	Structure confirmed

8762 #109 RT: 0.49 AV: 1 SB: 225 1.00 , 0.00-1.00 NL: 3.73E7
T: FTMS + p ESI Full ms [60.00-750.00]
103.08689





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



Results of Peak Find

No.	Position	Intensity
1	3413.39	87.6611
2	2872.45	81.0342
3	1668.12	71.2286
4	1618.95	81.8253
5	1488.78	75.7484
6	1343.18	87.0308
7	1264.11	88.0106
8	1139.72	86.1392
9	1029.8	84.6055
10	982.554	88.8735
11	841.776	94.0034
12	762.709	90.0578
13	673.035	83.8175

Revision table

Revision	Date	Reason for revision
00	30 Jul 2019	Release of the Certificate of Analysis - initial version

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