



Mikromol™



Certificate of Analysis

ISO 9001

Reference Material

Product name

Thieno[3,2-c]pyridine

Product code

MM0150.12

CAS number

272-14-0

Molecular weight

135.19

Molecular formula

C₇H₅NS

Lot number

1037473

Appearance

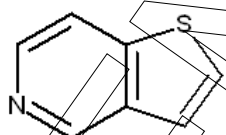
brown solid

Melting point (DSC)

50 °C

Long-term storage

2 to 8 °C, dark



Assay "as is"
99.2 %

Date of shipment:

03 Feb 2020

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, 31 Jan 2020		



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

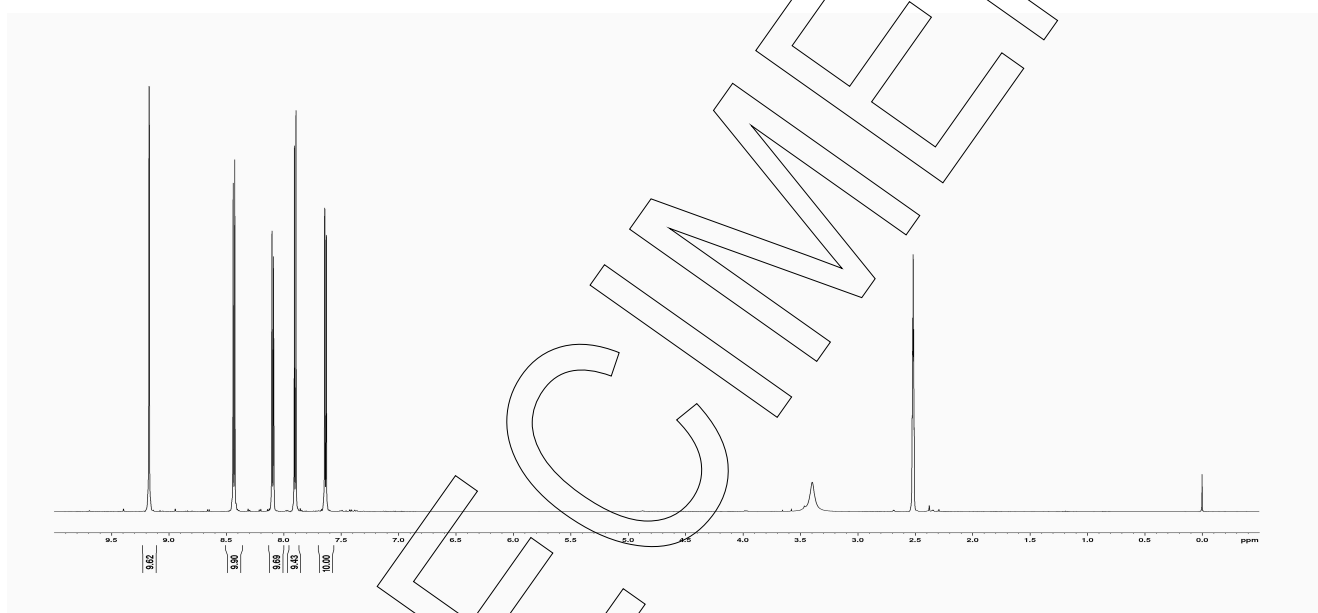
Revision table

SPECIMEN

Identity

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

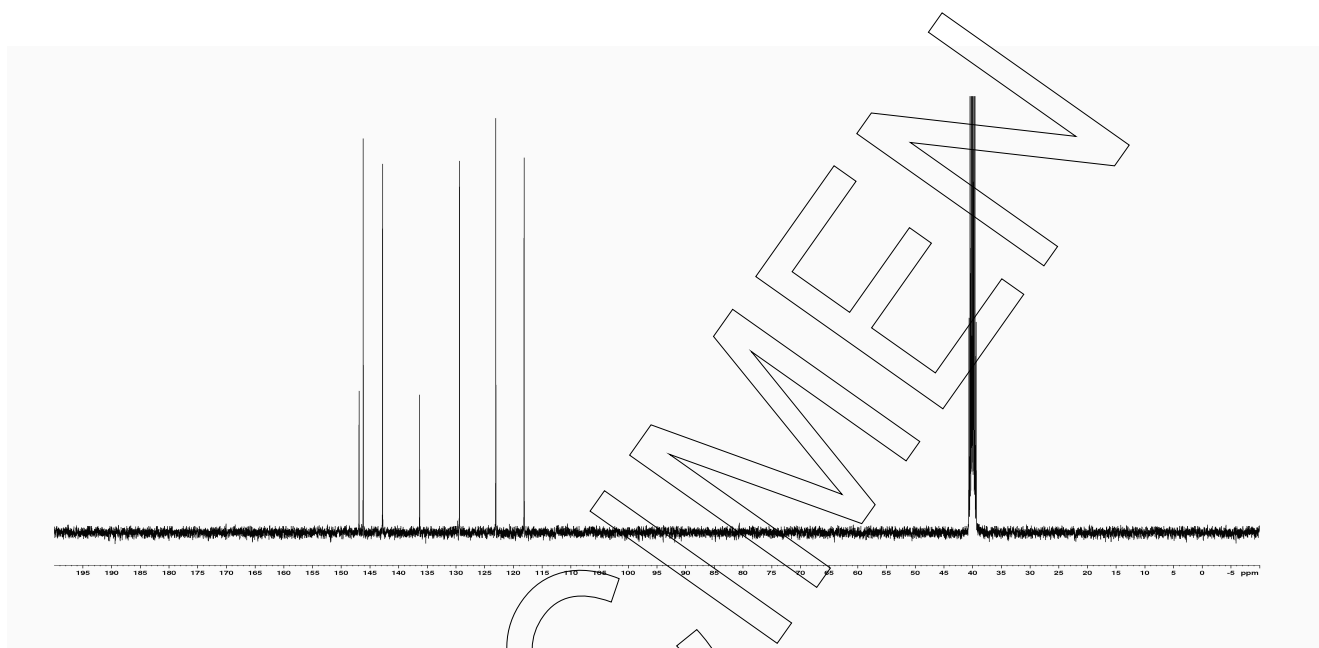
Method	Conditions	Result
$^1\text{H-NMR}$	400 MHz, DMSO-d_6	Structure confirmed





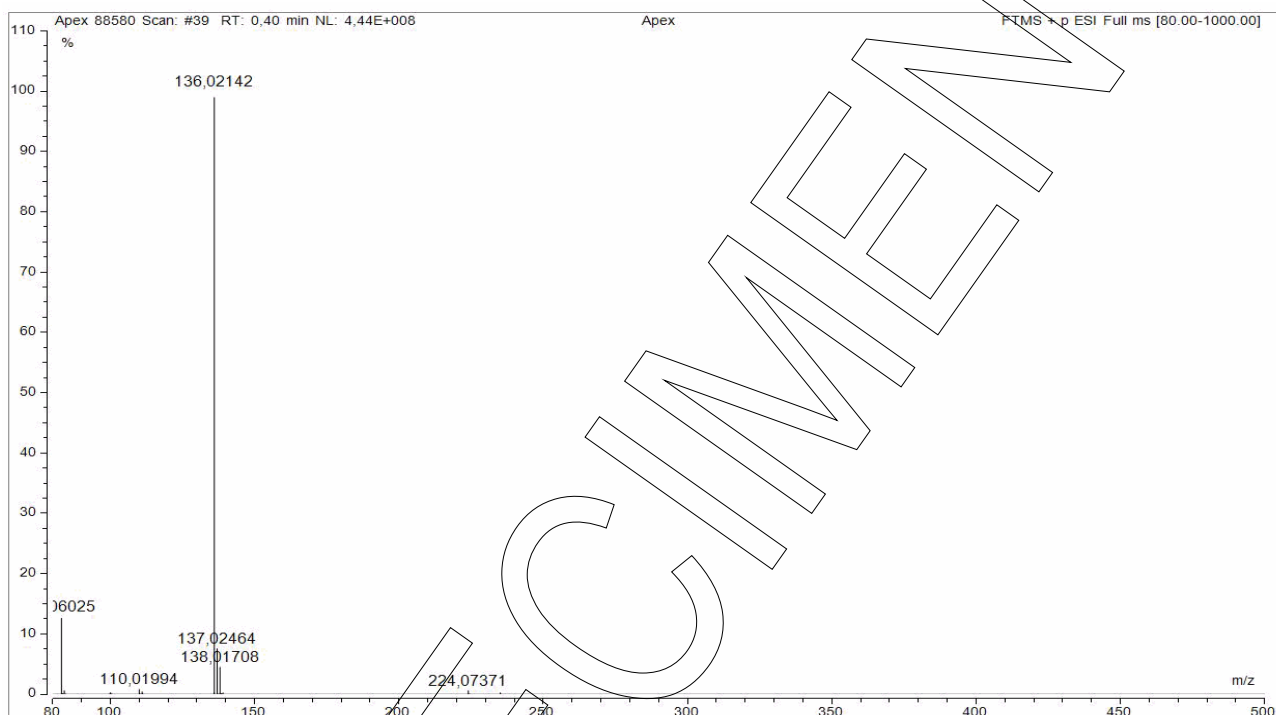
Mikromol™

Method	Conditions	Result
¹³ C-NMR	100 MHz, DMSO-d ₆	Structure confirmed



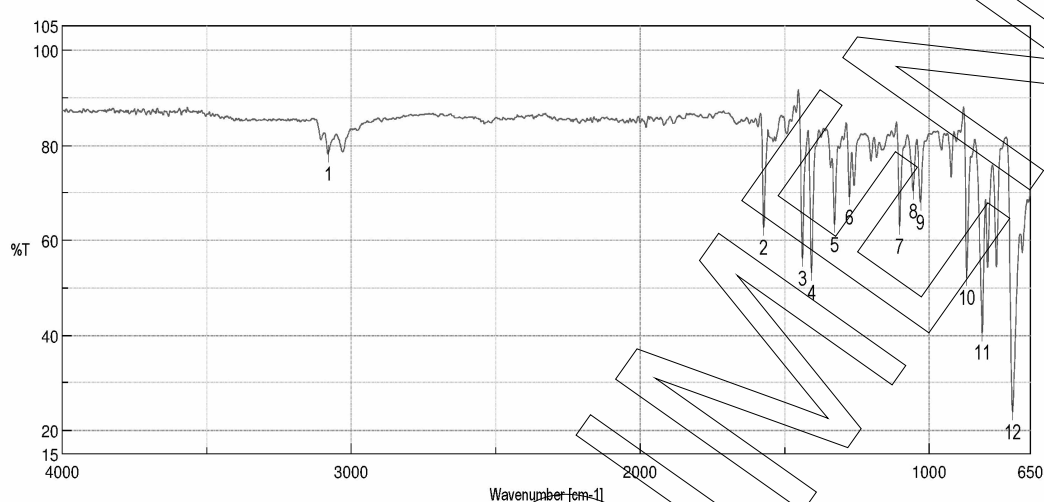


Method	Conditions	Result
MS	3.5 kV ESI+; capillary temperature: 269 °C Theoretical value: 136.02155	Structure confirmed





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



Results of Peak Find

No.	Position	Intensity
1	3079.76	78.2177
2	1572.66	62.666
3	1438.64	56.155
4	1406.82	53.2435
5	1327.75	63.309
6	1275.68	69.0201
7	1102.12	62.9013
8	1055.84	70.2739
9	1029.8	67.9372
10	870.703	52.1722
11	816.706	40.5146
12	711.604	23.8586



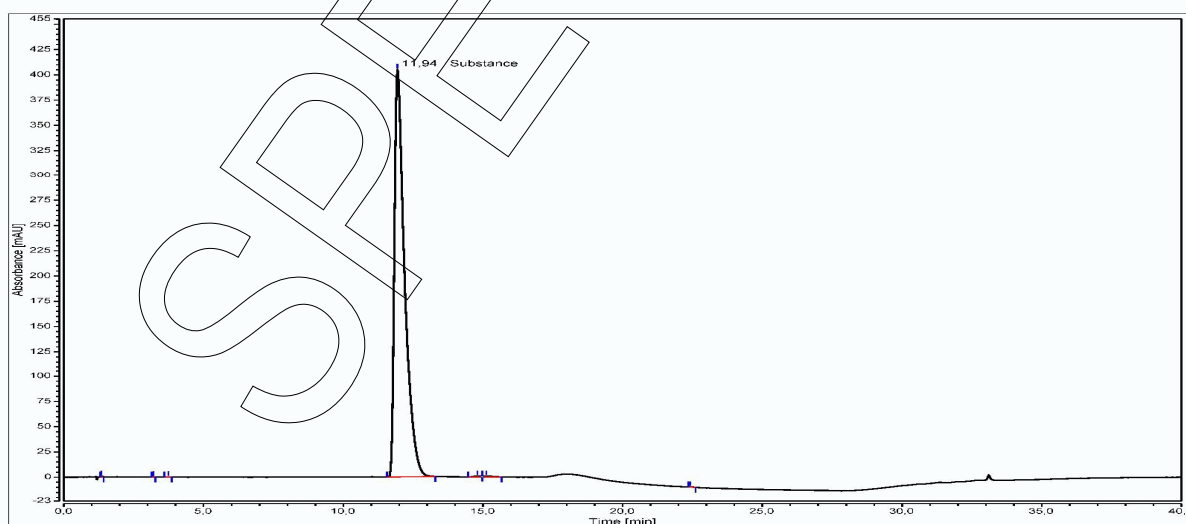
Assay

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

Purity by high performance liquid chromatography (HPLC)

HPLC Conditions:	
Column	Discovery HS F5, 3 µm, 150 x 4.0 mm
Column temperature	40 °C
Detector	DAD, 232 nm
Injector	Auto 2 µl; 0.0834 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	0-15 min A/B 15/85 15-20 min A/B to 60/40 20-25 min A/B 60/40 25-30 min A/B to 15/85 30-40 min A/B 15/85 (v/v)

HPLC chromatogram and peak table





Area percent report - sorted by signal

Pk #	Retention time	Area	Area %
1	1.343	0.0597	0.03
2	3.203	0.0214	0.01
3	3.740	0.0352	0.02
4	11.940	171.0735	99.55
5	14.802	0.2635	0.15
6	15.118	0.3685	0.21
7	22.412	0.0271	0.02
Totals		171.8489	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)

99.56 %; SD = 0.02 %

Volatile content

Water content

Method Karl Fischer titration

Result (n = 3) 0.38 %; SD = 0.03 %

Residual solvents

Method ¹H-NMR

Result (n = 1) No significant amounts of residual solvents were detected (< 0.05 %).



Final result

Assay "as is": 99.18 %

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	31 Jan 2020	Release of the Certificate of Analysis - initial version

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