

Certificate of Analysis

ISO 9001

Reference Material

Product name

2-Nitro-1-phenyl-1-propanol

Product code

MM0652.05

CAS number

6343-57-3

Molecular weight

181.19

Molecular formula

C₉H₁₁NO₃

Lot number

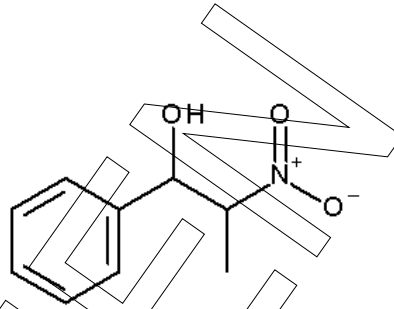
1030312

Appearance

colourless oil

Long-term storage

2 to 8 °C, dark



Assay "as is"
96.8 %

Date of shipment:

02 Dec 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, 15 Nov 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

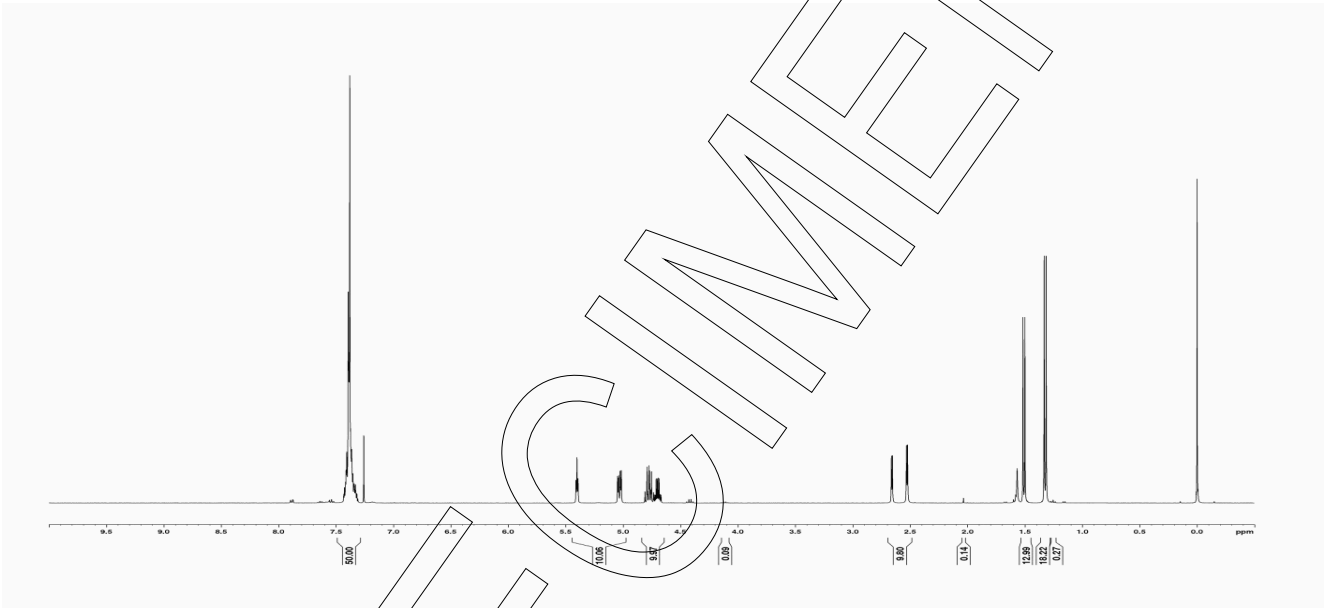
SPECIMEN



Identity

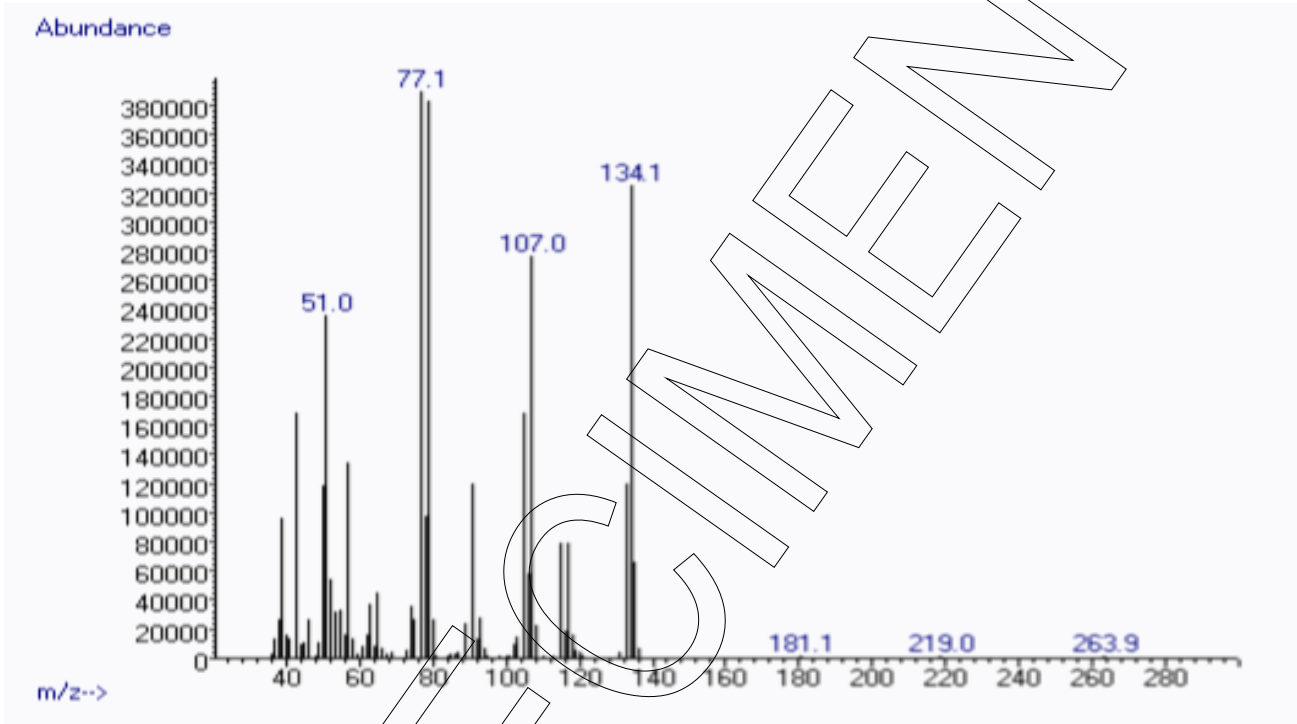
The identity of the reference material was established by following analyses.

Method	Conditions	Result
¹ H-NMR	400 MHz, CDCl ₃	Structure confirmed



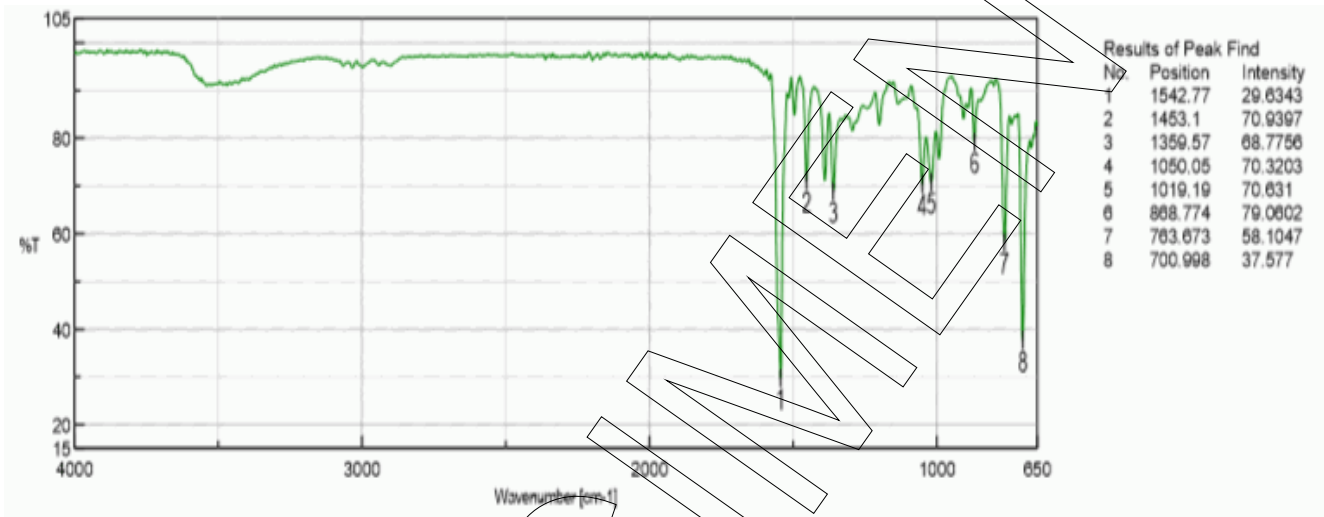


Method	Conditions	Result
MS	EI, 70eV, detector temperature: 280 °C	Structure confirmed





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



SPECIMEN



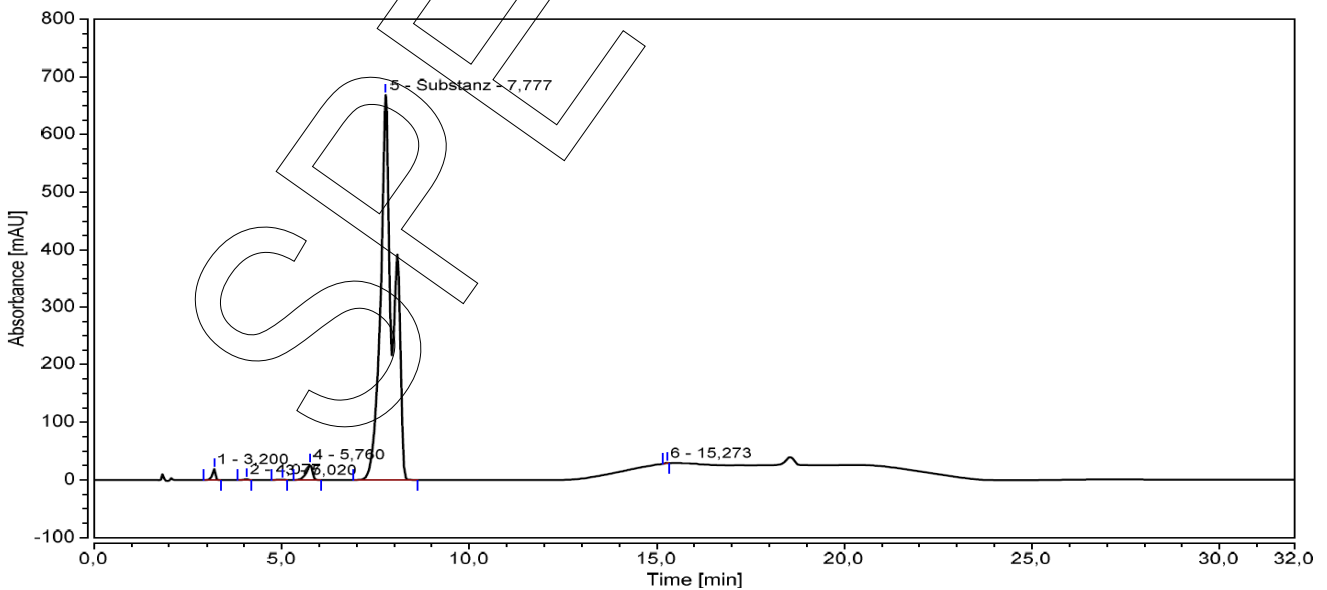
Assay

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, 210 nm
Injector	Auto 1.00 µl; 0.970 mg/ml in Methanol
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	0-10 min A/B 70/30 10-13 min A/B to 30/70 13-18 min A/B 30/70 18-21 min A/B to 70/30 21-32 min A/B 70/30 (v/v)

HPLC chromatogram and peak table





Area percent report - sorted by signal

Pk #	Retention time	Area	Area %
1	3.200	1.754	0.66
2	4.077	0.162	0.06
3	5.020	0.041	0.02
4	5.760	4.887	1.84
5	7.777	259.120	97.39
6	15.273	0.102	0.04
Totals		266.066	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)

97.36 %, SD = 0.03 %

Volatile content

Water content

Method Karl Fischer titration

Result (n = 3) 0.39 %; SD = 0.03 %

Residual solvents

Method ¹H-NMR

Result (n = 1) Sum: 0.23 %

0.23 % Ethyl acetate



Final result

Assay "as is": 96.76 %

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	15 Nov 2019	Release of the Certificate of Analysis - initial version

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