



Certificate of Analysis

ISO 9001

Reference Material

Product name

1-Cyclopropyl-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylic Acid (Desfluoro Compound)

Product code

MM0018.05-0025

CAS number

93107-11-0

Molecular weight

313.35

Molecular formula

C₁₇H₁₉N₃O₃

Lot number

1147548

Appearance

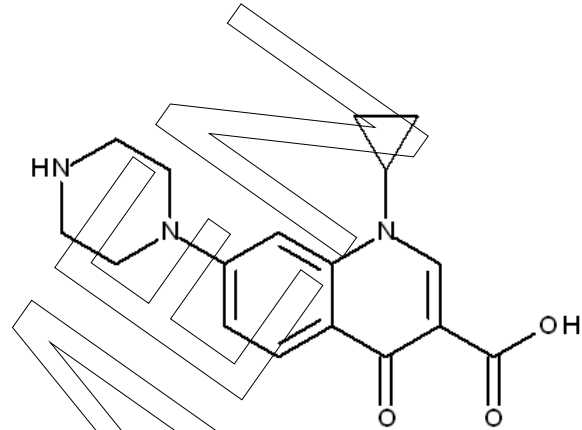
pale yellow solid

Melting point (DSC)

293 °C

Long-term storage

2 to 8 °C, dark
hygroscopic



Assay "as is"
93.2 %

Date of shipment:

20 Jul 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, 28 Jun 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

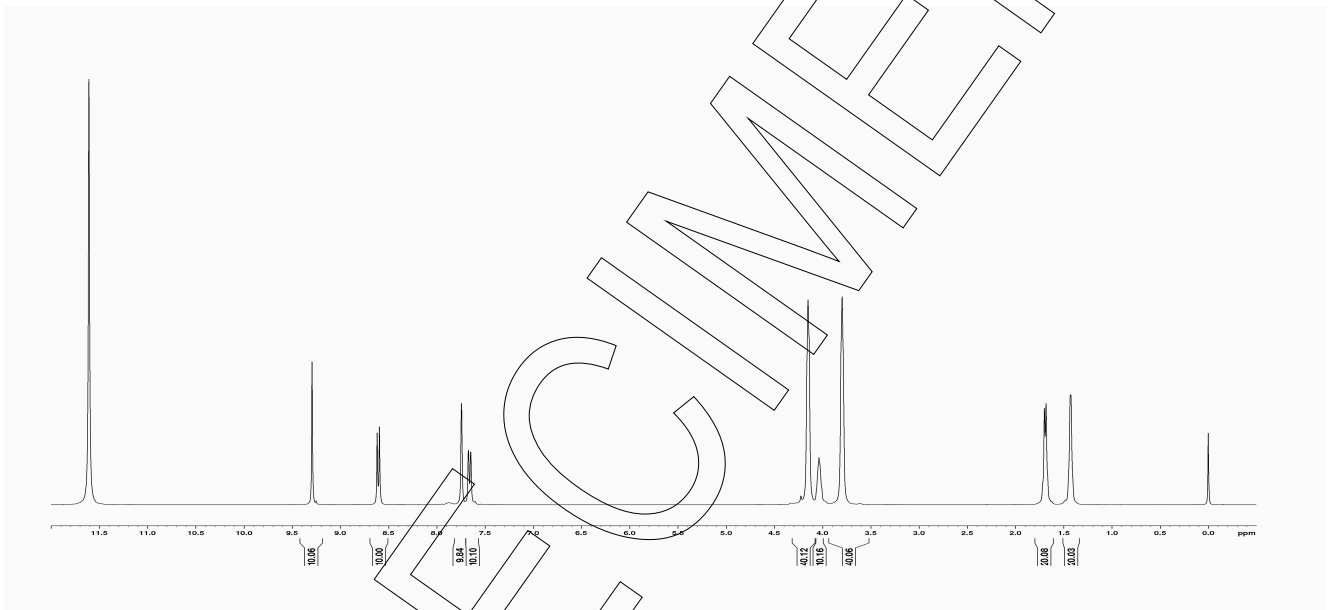
SPECIMEN



Identity

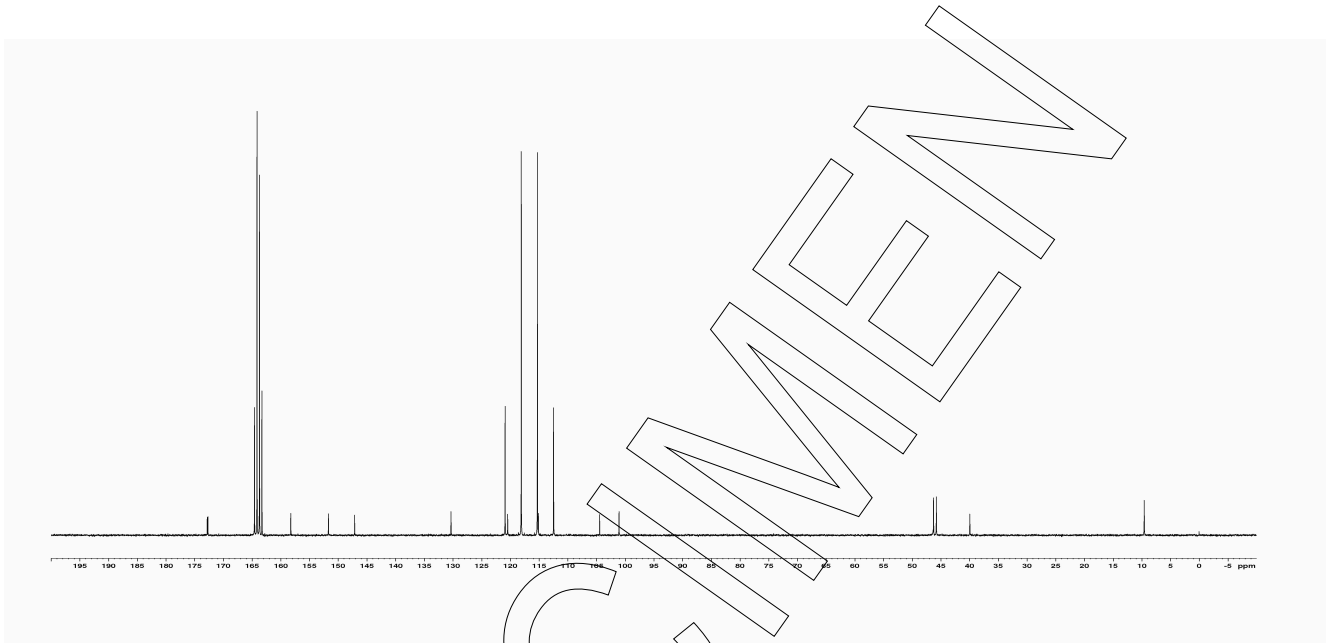
The identity of the reference material was established by following analyses.

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



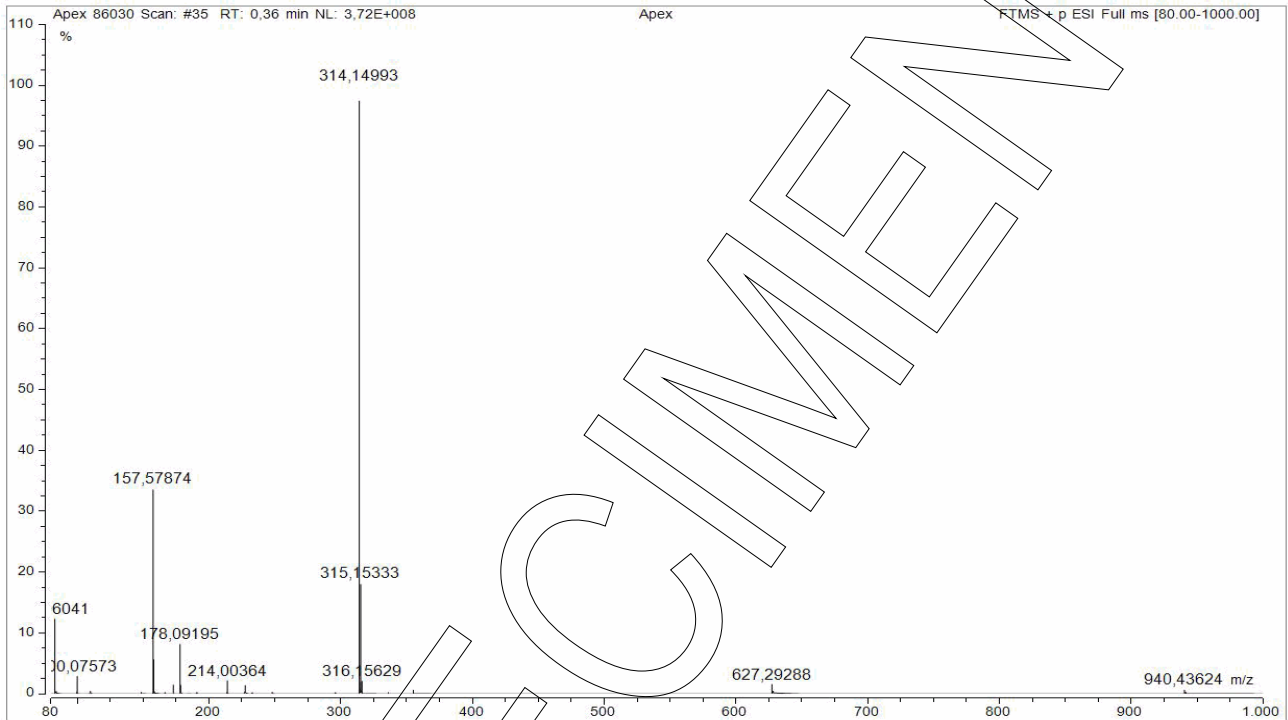


Method	Conditions	Result
¹³ C-NMR	100 MHz, CF ₃ COOD	Structure confirmed





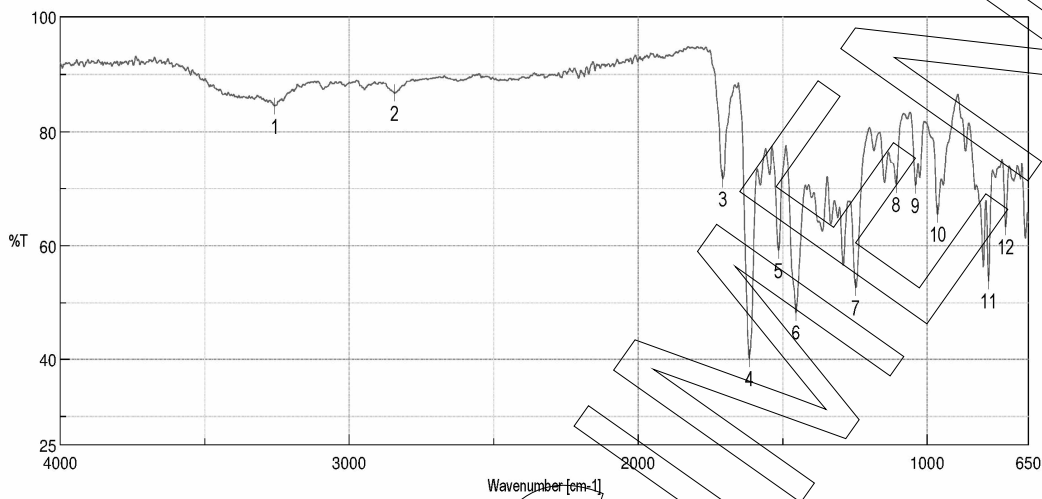
Method	Conditions	Result
MS	3.5 kV ESI+; capillary temperature: 269 °C Theoretical value: 314.14992	Structure confirmed



SPECIMEN



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



Results of Peak Find

No.	Position	Intensity
1	3257.18	84.4609
2	2842.56	86.7453
3	1706.69	71.5981
4	1616.06	40.0556
5	1513.85	59.1059
6	1454.06	48.2395
7	1246.75	52.6282
8	1106.94	70.6213
9	1040.41	70.5092
10	964.233	65.4578
11	787.779	53.809
12	728.961	63.2425



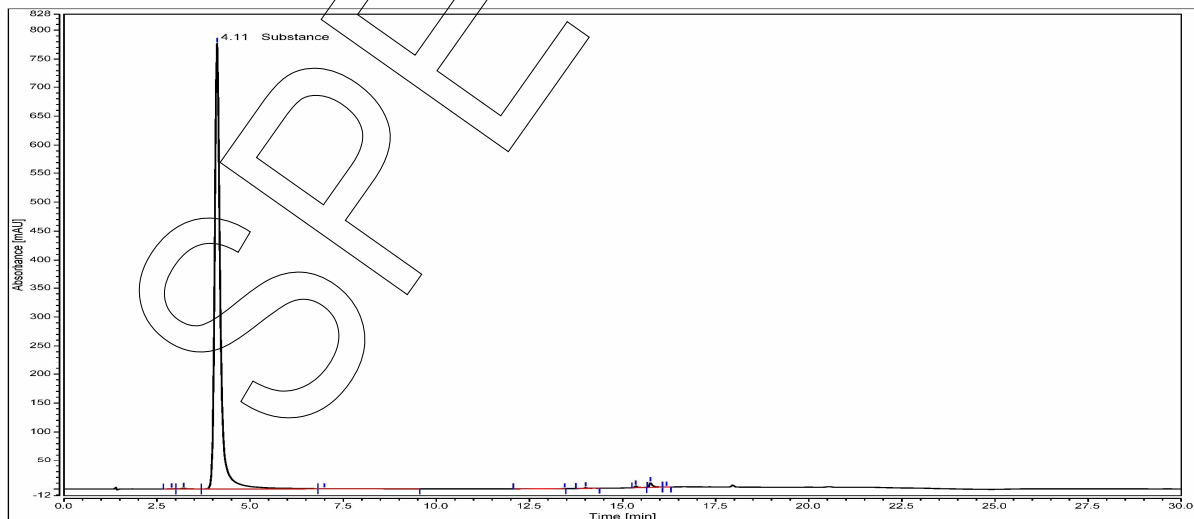
Assay

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

Purity by high performance liquid chromatography (HPLC)

HPLC Conditions:	
Column	LiChrospher 60 RP-select B; 5 µm, 125 x 4.0 mm
Column temperature	40 °C
Detector	DAD, 280 nm
Injector	Auto 3 µl; 0.0536 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	0-10 min A/B 85/15 10-15 min A/B to 30/70 15-20 min A/B 30/70 20-23 min A/B to 85/15 23-30 min A/B 85/15 (v/v)

HPLC chromatogram and peak table





Area percent report - sorted by signal

Pk #	Retention time	Area	Area %
1	2.888	0.0467	0.03
2	3.217	0.2288	0.16
3	4.113	137.7098	98.45
4	6.998	0.5446	0.39
5	13.450	0.0830	0.06
6	14.010	0.1333	0.10
7	15.352	0.2510	0.18
8	15.750	0.8434	0.60
9	16.183	0.0362	0.03
Totals		139.8768	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) 98.43 %; SD = 0.02 %

Volatile content

Water content

Method Karl Fischer titration
Result (n = 3) 5.30 %; SD = 0.20 %

Residual solvents

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



Final result

Assay "as is": 93.21 %

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	28 Jun 2021	Release of the Certificate of Analysis - initial version

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