

Certificate of Analysis

Reference Material

Product name

(Z)-(2,4-Difluorophenyl)-(4-piperidyl)methanone Oxime

Product code

MM0491.28-0025

CAS number

691007-05-3

Molecular weight

240.25

Molecular formula

C₁₂H₁₄F₂N₂O

Lot number

1221223

Appearance

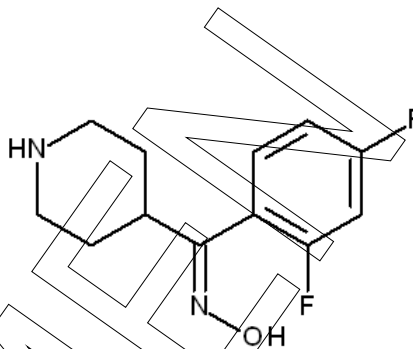
white solid

Melting point

> 192 °C (dec.)

Long-term storage

2 to 8 °C, dark



Assay "as is"
98.9 %

Date of shipment:

30 Aug 2022

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, 28 Feb 2022		



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

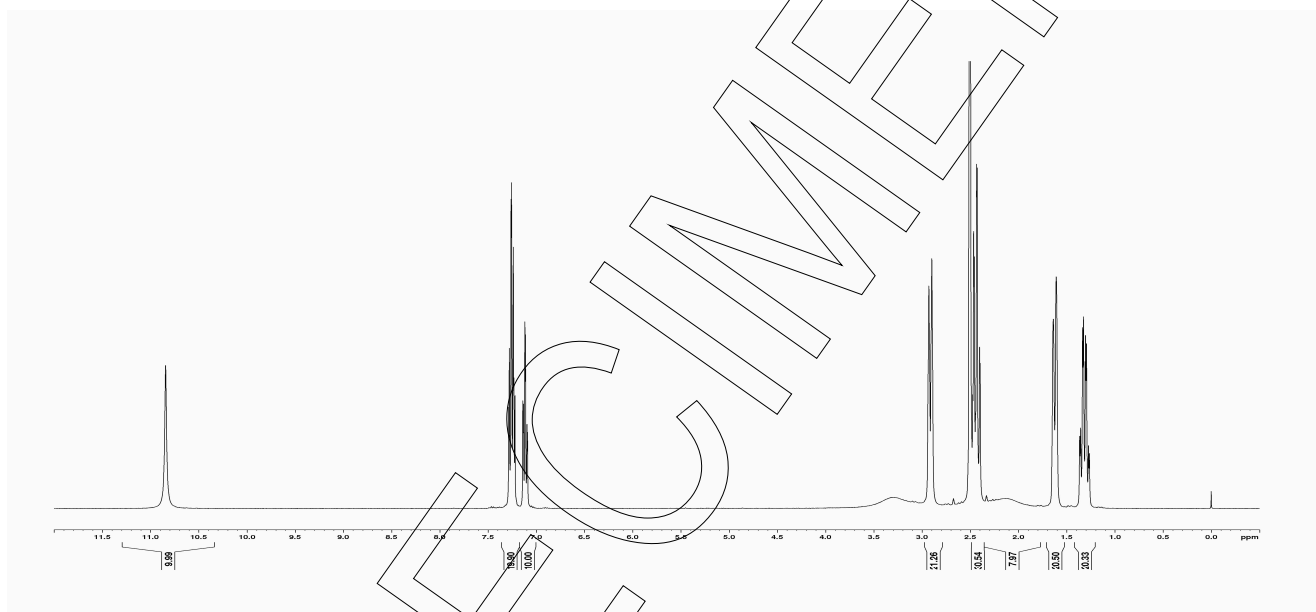
SPECIMEN



Identity

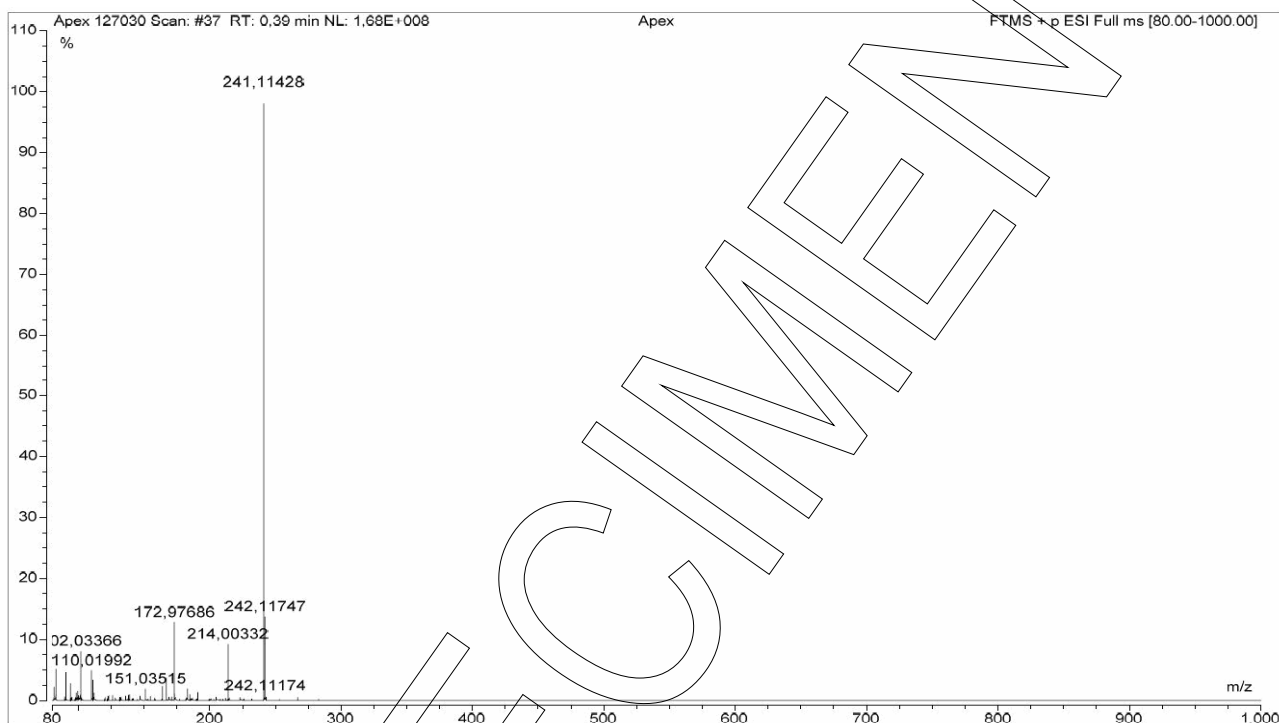
The identity of the reference material was established by following analyses.

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



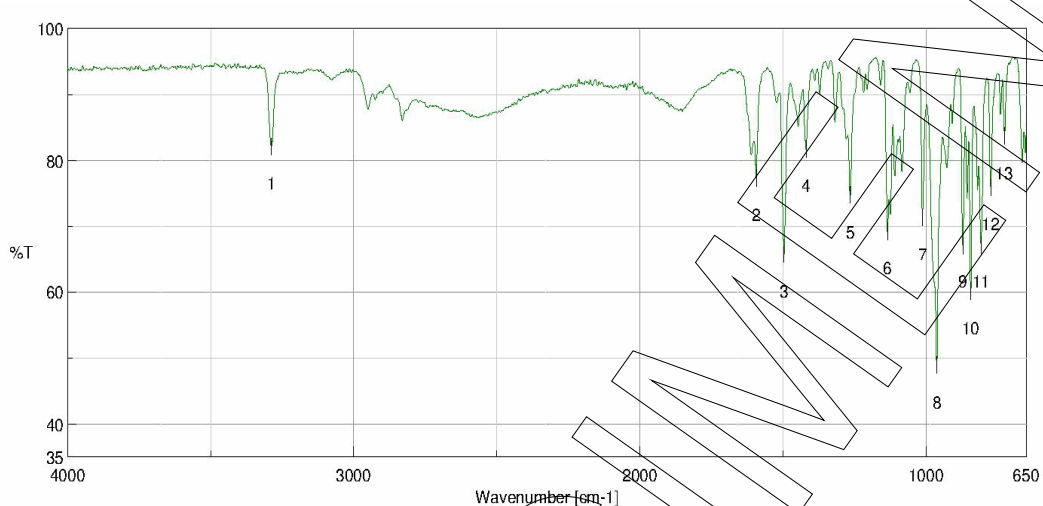


Method	Conditions	Result
MS	3.5 kV ESI+; capillary temperature: 269 °C Theoretical value: 241.11470	Structure confirmed





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



Results of Peak Find		
No.	Position	Intensity
1	3287.07	82.1407
2	1592.91	77.3521
3	1496.49	65.6902
4	1419.35	81.7488
5	1265.07	74.7379
6	1133.94	69.1779
7	1012.45	71.3617
8	962.305	48.9091
9	870.703	67.0913
10	843.704	60.0273
11	807.063	67.1349
12	773.315	75.9484
13	726.068	83.729



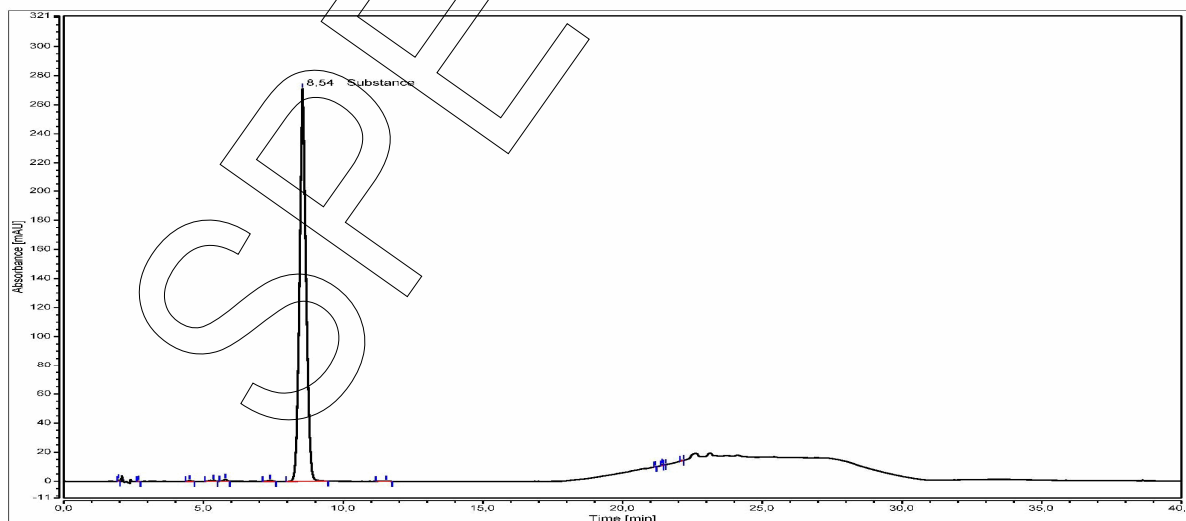
Assay

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, 220 nm
Injector	Auto 2 µl; 0.3422 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	0-15 min A/B 90/10 15-20 min A/B to 50/50 20-25 min A/B 50/50 25-28 min A/B to 90/10 28-40 min A/B 90/10 (v/v)

HPLC chromatogram and peak table





Area percent report - sorted by signal

Pk #	Retention time	Area	Area %
1	1.962	0.0421	0.06
2	2.682	0.0067	0.01
3	4.508	0.0702	0.10
4	5.357	0.1697	0.23
5	5.780	0.2065	0.28
6	7.380	0.1485	0.20
7	8.542	72.2871	98.87
8	11.532	0.0975	0.13
9	21.170	0.0145	0.02
10	21.418	0.0367	0.05
11	21.540	0.0104	0.01
12	22.190	0.0232	0.03
Totals		73.1131	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)

98.87 %; SD = 0.01 %

Volatile content

Water content

Method

Karl Fischer titration

Result (n = 3)

No significant amounts of water were detected (< 0.05 %).



Residual solvents

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

Final result

Assay "as is": 98.87 %

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 Feb 2022	Release of the Certificate of Analysis - initial version

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