



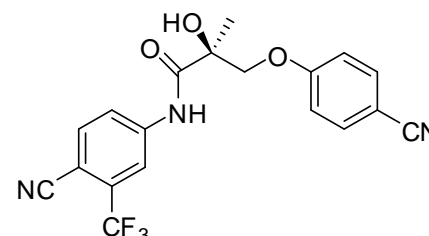
CERTIFIED REFERENCE MATERIAL CERTIFICATE OF ANALYSIS

NMIA D1075: Ostarine

Report ID: D1075.2023.01

Chemical Formula: C₁₉H₁₄F₃N₃O₃

Molecular Weight: 389.3 g/mol



Certified value

Batch No.	CAS No.	Purity (mass fraction)
20-D-04	841205-47-8	96.2 ± 1.5%

The uncertainty has been calculated according to ISO Guide 35 and is stated at the 95% confidence limit ($k = 2$).

IUPAC name: (2S)-3-(4-Cyanophenoxy)-N-[4-cyano-3-(trifluoromethyl)phenyl]-2-hydroxy-2-methylpropanamide. The stereochemistry of the main component detailed in the structure above and the IUPAC name is based on literature precedents and has not been verified for this material. The enantiomeric purity of this material has also not been verified.

Expiration of certification: The property values are valid till 18 January 2026, i.e. three years from the date of re-certification provided the **unopened** material is handled and stored in accordance with the recommendations below. The material as issued in the unopened container and stored as recommended below should be suitable for use beyond this date, subject to confirmation of batch stability from the issuing body. The expiry date/shelf life does not apply to sample bottles that have been opened. In such cases it is recommended that the end-user conduct their own in-house stability trials. The material will be re-tested on an annual basis to ensure that the property values are still valid. In the event a product fails the stability trial, notification will be sent to all impacted customers.

Description: Off-white powder sourced from an external supplier, and certified for identity and purity by NMIA. Packaged in amber glass bottles with a septum and crimped aluminium cap.

Intended use: This certified reference material is suitable for use as a primary calibrator.

Instructions for use: Equilibrate the bottled material to room temperature before opening.

Recommended storage: When not in use this material should be stored at or below 25 °C in a closed container in a dry, dark area.

Metrological traceability: The certified purity value is traceable to the SI unit for mass (kg) through Australian national standards via balance calibration. In the mass balance approach all impurities are quantified as a mass fraction and subtracted from 100%.

Stability: In the absence of long term stability data the measurement uncertainty at the 95% coverage interval has been expanded to accommodate any potential change in the property value. The stability component has been estimated from stability trials conducted on similar materials by NMI Australia over the last ten years. In the absence of long term stability data the measurement uncertainty at the 95% coverage interval has been expanded to accommodate any potential change in the property value. The stability component has been estimated from short term accelerated stability trials. The long-term stability of the compound in solution has not been examined.

Homogeneity assessment: The homogeneity of the material was assessed using purity assay by HPLC with UV detection on ten randomly selected 1-2 mg sub samples of the material. The material was judged to be sufficiently homogeneous at this level of sampling as the variation in analysis results between samples was not significantly different at a 95% confidence level from that observed on repeat analysis of the same sample.

Safety: Treat as a hazardous substance. Use appropriate work practices when handling to avoid skin or eye contact, ingestion or inhalation of dust. Refer to the provided safety data sheet.

S. R. Davies

Dr Stephen R. Davies,
Team Leader,
Chemical Reference Materials, NMI.
25 January 2023

This report supersedes any issued prior to 25 January 2023

NATA Accreditation No. 198 / Corporate Site No. 14214.

Legal notice: Terms and Conditions associated with the provision of this reference material can be found on the NMIA website.

Characterisation Report:

The identity was confirmed by a range of spectroscopic techniques, NMR, IR and MS. The certified purity value was obtained from a combination of traditional analytical techniques. The techniques used in the mass balance approach include HPLC with UV detection, thermogravimetric analysis, Karl Fischer analysis, and ¹H NMR spectroscopy. The purity value is calculated as per Equation 1.

$$\text{Purity} = (100\% - I_{\text{ORG}}) \times (100\% - I_{\text{VOL}} - I_{\text{NVR}}) \quad \text{Equation 1}$$

I_{ORG} = Organic impurities of related structure, I_{VOL} = volatile impurities, I_{NVR} = non-volatile residue

Supporting evidence is provided by elemental microanalysis.

HPLC:	Instrument:	Shimadzu Binary pump LC-20AB, SIL-20 A HT auto sampler
	Column:	Alltima C-18, 5 μm (4.6 mm x 150 mm)
	Column oven:	40 $^{\circ}\text{C}$
	Mobile Phase:	A = Milli-Q water; B = Acetonitrile 0-20 min 50% B; 20-25 min 50-80% B; 25-28 min 80% B; 28-30 min 80-50% B, 30-45 min 50% B.
	Flow rate:	1.0 mL/min
	Detector:	Shimadzu SPD-M20A PDA operating at 250 nm
	Relative mass fraction of the main component:	
	Initial analysis:	Mean = 99.9%, s = 0.004% (10 sub samples in duplicate, February 2021)
	Re-analysis:	Mean = 99.8%, s = 0.03% (5 sub samples in duplicate, January 2022)
	Re-analysis:	Mean = 99.9%, s = 0.003% (5 sub samples in duplicate, January 2023)
Karl Fischer analysis:	Moisture content	0.2-0.3% mass fraction (February 2021) 0.4% mass fraction (December 2021) <0.1% mass fraction (October 2022)
Thermogravimetric analysis:	Non-volatile residue	< 0.2% mass fraction (February 2021)

Spectroscopic and other characterisation data

ESI-MS:	Instrument:	Waters Acquity TQ API mass spectrometer
	Operation:	Positive ion mode, direct infusion at 10 μ L/min
	Ionisation:	ESI spray voltage at 3.0 kV positive ion
	EM voltage:	650 V
	Cone voltage:	30 V
	Peak:	412 (M+Na ⁺) <i>m/z</i>
IR:	Instrument:	Bruker Alpha Platinum ATR
	Range:	4000-400 cm^{-1} , neat
	Peaks:	3407, 3329, 2224, 1687, 1605, 1508, 1428, 1326, 1260, 1171, 1134, 1035, 902, 837, 673, 547 cm^{-1}
¹ H NMR:	Instrument:	Bruker Avance III-500
	Field strength:	500 MHz
	Solvent:	DMSO- <i>d</i> ₆ (2.50 ppm)
	Spectral data:	δ 1.45 (3H, s), 4.09 (1H, d, <i>J</i> = 9.5 Hz), 4.33 (1H, d, <i>J</i> = 9.5 Hz), 6.37 (1H, br s), 7.10 (2H, d, <i>J</i> = 8.9 Hz), 7.73 (2H, d, <i>J</i> = 8.9 Hz), 8.09 (1H, d, <i>J</i> = 8.5 Hz), 8.29 (1H, dd, <i>J</i> = 2.0, 8.5 Hz), 8.54 (1H, d, <i>J</i> = 2.0 Hz), 10.59 (1H, br s) ppm Benzene estimated at 3.7% mass fraction was observed in the ¹ H NMR.
¹³ C NMR:	Instrument:	Bruker Avance III-500
	Field strength:	126 MHz
	Solvent:	DMSO- <i>d</i> ₆ (39.52 ppm)
	Spectral data:	δ 23.0, 73.8, 74.8, 102.1 (<i>J</i> _{CF} = 2.0 Hz), 103.1, 115.8, 115.9, 117.5 (<i>J</i> _{CF} = 5.0 Hz), 119.1, 122.5 (<i>J</i> _{CF} = 272.9 Hz), 122.8, 131.6 (<i>J</i> _{CF} = 31.4 Hz), 134.2, 136.4, 143.2, 161.9, 174.4 ppm
Melting point:		129-131 °C
Microanalysis:	Found:	C = 59.6%; H = 3.8%; N = 10.4% (March, 2021)
	Calculated:	C = 58.6%; H = 3.6%; N = 10.8% (Calculated for C ₁₉ H ₁₄ F ₃ N ₃ O ₃)
	Calculated:	C = 59.9%; H = 3.8%; N = 10.4% (Calculated for C ₁₉ H ₁₄ F ₃ N ₃ O ₃ · 0.2C ₆ H ₆)