

# **Certificate of Analysis**

Print Date: Oct 28th 2022

www.tocris.com

Product Name: Nutlin 3a Catalog No.: 6075 Batch No.: 1

CAS Number: 675576-98-4

IUPAC Name: 4-[[(4S,5R)-4,5-Bis(4-chlorophenyl)-4,5-dihydro-2-[4-methoxy-2-(1-methylethoxy)phenyl]-1H-imidazol-1-yl]carbonyl]-

2-piperazinone

# 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{30}H_{30}Cl_2N_4O_4.\frac{1}{2}H_2O$ 

Batch Molecular Weight: 590.5

Physical Appearance: White solid

**Solubility:** DMSO to 100 mM

ethanol to 100 mM

Storage: Store at -20°C

**Batch Molecular Structure:** 

# 2. ANALYTICAL DATA

HPLC: Shows 97.2% purity
Chiral HPLC: Shows 100% purity

<sup>1</sup>H NMR: Consistent with structure Mass Spectrum: Consistent with structure

**Optical Rotation:**  $[\alpha]_D = -131.3$  (Concentration = 0.13, Solvent = Chloroform)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 61.02 5.29 9.49 Found 61.03 5 9.54

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use



# **Product Information**

Print Date: Oct 28th 2022

www.tocris.com

Product Name: Nutlin 3a Catalog No.: 6075 1

CAS Number: 675576-98-4

IUPAC Name: 4-[[(4S,5R)-4,5-Bis(4-chlorophenyl)-4,5-dihydro-2-[4-methoxy-2-(1-methylethoxy)phenyl]-1*H*-imidazol-1-yl]carbonyl]-

2-piperazinone

#### **Description:**

Nutlin 3a is an MDM2 antagonist ( $IC_{50}$  = 90 nM); inhibits the MDM2-p53 interaction. Active enantiomer of Nutlin-3 (Cat. No. 3984). Induces expression for P53 regulated genes. Suppresses tumor growth in vivo >98% in prostate cancer and osteosarcoma cancer models. Antiproliferative.

#### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>30</sub>H<sub>30</sub>Cl<sub>2</sub>N<sub>4</sub>O<sub>4</sub>.½H<sub>2</sub>O

Batch Molecular Weight: 590.5 Physical Appearance: White solid

**Minimum Purity:** ≥97%

# **Batch Molecular Structure:**

Storage: Store at -20°C

# Solubility & Usage Info:

DMSO to 100 mM ethanol to 100 mM

#### Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

### References:

**Tovar** *et al* (2006) Small-molecule MDM2 antagonists reveal aberrant p53 signaling in cancer: implications for therapy. Proc.Natl.Acad.Sci.USA. *103* 1888. PMID: 16443686.

Vassilev et al (2004) In vivo activation of the p53 pathway by small-molecule antagonists of MDM2. Science 303 844. PMID: 14704432.