

Certificate of Analysis

Print Date: Nov 16th 2018

www.tocris.com

Product Name: BYK 49187 Catalog No.: 3735 Batch No.: 1

CAS Number: 163120-31-8

IUPAC Name: 4,5-Dihydro-2-[4-(4-methyl-1*H*-imidazol-4-yl)-1-piperidinyl]-6*H*-imidazo[4,5,1-*ij*]quinolin-6-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{19}H_{21}N_5O$

Batch Molecular Weight: 335.4

Physical Appearance: Beige solid

Solubility: DMSO to 10 mM

ethanol to 50 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.35$ (Dichloromethane:Methanol [10:1])

HPLC: Shows 98.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Tel: +44 (0)1235 529449 www.tocris.com/distri Tel:+1 612 379 2956



Product Information

Print Date: Nov 16th 2018

www.tocris.com

Product Name: BYK 49187 Catalog No.: 3735 Batch No.: 1

CAS Number: 163120-31-8

IUPAC Name: 4,5-Dihydro-2-[4-(4-methyl-1*H*-imidazol-4-yl)-1-piperidinyl]-6*H*-imidazo[4,5,1-*ij*]quinolin-6-one

Description:

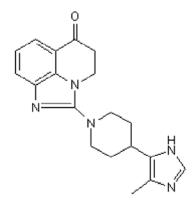
PARP-1 and PARP-2 inhibitor (pIC $_{50}$ values are 8.36 and 7.50 for cell-free recombinant PARP-1 and murine PARP-2 respectively). Displays potent inhibitory activity against human PARP-1 in cell-free and cellular assays in vitro; reduces myocardial infarct size in vivo.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{19}H_{21}N_5O$ Batch Molecular Weight: 335.4 Physical Appearance: Beige solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 10 mM ethanol to 50 mM

This product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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:

Sunderland *et al* (2011) 5-Benzamidoisoquinolin-1-ones and 5-(omega-carboxyalkyl)isoquinolin-1-ones as isoform-selective inhibitors of poly(ADP-ribose) polymerase 2 (PARP-2). J.Med.Chem. *54* 2049. PMID: 21417348.

Eltze et al (2008) Imidazoquinolinone, imidazopyridine, and isoquinolindione derivatives as novel and potent inhibitors of the poly(ADP-ribose) polymerase (PARP): a comparison with standard PARP inhibitors. Mol.Pharmacol. 74 1587. PMID: 18809672.