

www.tocris.com

Print Date: Jan 14th 2016

TOCRIS a biotechne brand

Product Name: EB 47 Catalog No.: 4140 Batch No.: 1

Certificate of Analysis

CAS Number: 1190332-25-2

IUPAC Name: 5'-Deoxy-5'-[4-[2-[(2,3-Dihydro-1-oxo-1H-isoindol-4-yl)amino]-2-oxoethyl]-1-piperazinyl]-5'-oxoadenosine

dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{24}H_{27}N_9O_6.2HCI.3H_2O$

Batch Molecular Weight: 664.5 **Physical Appearance:** White solid

Solubility: water to 5 mM with gentle warming

DMSO to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.4% purity

1H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

wass spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 43.38 5.31 18.97 Found 43.26 5.37 18.95



Product Information

Print Date: Jan 14th 2016

www.tocris.com

Product Name: EB 47 Catalog No.: 4140 Batch No.: 1

CAS Number: 1190332-25-2

IUPAC Name: 5'-Deoxy-5'-[4-[2-[(2,3-Dihydro-1-oxo-1H-isoindol-4-yl)amino]-2-oxoethyl]-1-piperazinyl]-5'-oxoadenosine

dihydrochloride

Description:

Potent inhibitor of PARP-1 ($IC_{50} = 45$ nM). Reduces infarct volume in both a rat transient middle cerebral arterial occlusion model and a cardiac reperfusion model.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{24}H_{27}N_9O_6.2HCI.3H_2O$

Batch Molecular Weight: 664.5 Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

water to 5 mM with gentle warming

DMSO to 50 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:

Jagtap *et al* (2004) The discovery and synthesis of novel adenosine substituted 2,3-dihydro-1*H*-isoindol-1-ones: potent inhibitors of poly (ADP-ribose) polymerase-1 (PARP-1). Bioorg.Med.Chem.Lett. **14** 81. PMID: 14684303.

Gaymes et al (2009) Inhibitors of poly ADP-ribose polymerase (PARP) induce apoptosis of myeloid leukemic cells: potential for therapy of myeloid leukemia and myelodysplastic syndromes. Haematologica **94** 638. PMID: 19407318.

Ferraris et al (2010) Evolution of poly(ADP-ribose) polymerase-1 (PARP-1) inhibitors. From concept to clinic. J.Med.Chem. 53 4561. PMID: 20364863.