

Product Name: A12B4C3

Catalog No.: 5097

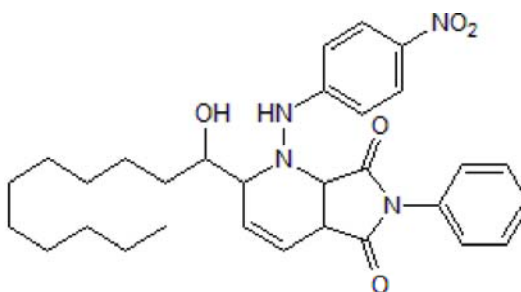
Batch No.: 1

CAS Number: 1005129-80-5

IUPAC Name: 4a,7a-Dihydro-2-(1-hydroxyundecyl)-1-[(4-nitrophenyl)amino]-6-phenyl-1*H*-pyrrolo[3,4-*b*]pyridine-5,7(2*H*,6*H*)-dione

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₀H₃₈N₄O₅
Batch Molecular Weight: 534.65
Physical Appearance: Yellow solid
Solubility: DMSO to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.3 (Ethyl acetate:Petroleum ether [2:1])
HPLC: Shows 98.9% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	67.39	7.16	10.48
Found	67.41	7.14	10.52

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

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Description:

Potent and selective polynucleotide kinase/phosphatase (PNKP) inhibitor (IC₅₀ = 60 nM). Displays no effect on calcineurin, protein PP-1 or APTX. Interrupts DNA repair and enhances radiosensitivity of human A549 lung carcinoma and MDA-MB-231 cells.

Physical and Chemical Properties:

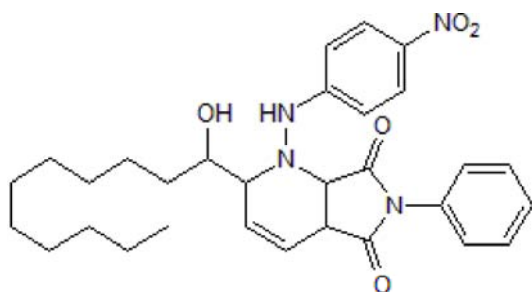
Batch Molecular Formula: C₃₀H₃₈N₄O₅

Batch Molecular Weight: 534.65

Physical Appearance: Yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO 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:

Schellenberg et al (2011) DNA end processing by polynucleotide kinase/phosphatase. *Proc.Natl.Acad.Sci.U.S.A.* **108** 20855. PMID: 22184240.

Freschauf et al (2010) Mechanism of action of an imidopiperidine inhibitor of human polynucleotide kinase/phosphatase. *J.Biol.Chem.* **285** 2351. PMID: 19940137.

Freschauf et al (2009) Identification of a small molecule inhibitor of the human DNA repair enzyme polynucleotide kinase/phosphatase. *Cancer Res.* **69** 7739. PMID: 19773431.

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