

Product Name: BX 795

Catalog No.: 4318

Batch No.: 2

CAS Number: 702675-74-9

IUPAC Name: *N*-[3-[[5-Iodo-4-[[3-[(2-thienylcarbonyl)amino]propyl]amino]-2-pyrimidinyl]amino]phenyl]-1-pyrrolidinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₂₆IN₇O₂S.¼H₂O

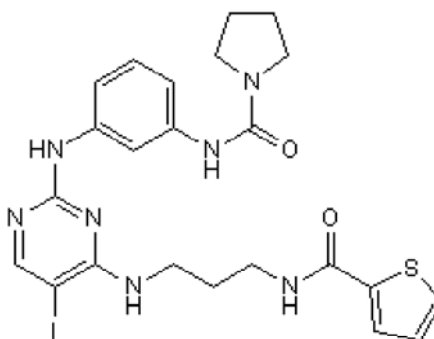
Batch Molecular Weight: 595.97

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.63 (Ethyl acetate)

HPLC: Shows 99.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	46.35	4.48	16.45
Found	46.09	4.54	16.29

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

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Description:

Inhibitor of 3-phosphoinositide-dependent kinase 1 (PDPK1). Inhibits Akt phosphorylation at Thr308 in PC3 cells; also inhibits anchorage-independent growth of PC3 and MDA-MB-468 cells. Exhibits activity at other kinases, including TANK-binding kinase 1 (TBK1), Aurora B and IκB kinase ε (IKKε). Also enhances lentiviral transduction of natural killer (NK) cells by around 3.8-fold.

Physical and Chemical Properties:

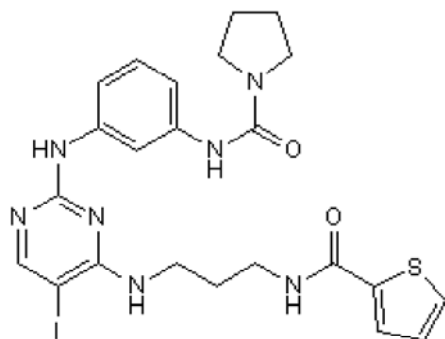
Batch Molecular Formula: C₂₃H₂₆IN₇O₂S·¼H₂O

Batch Molecular Weight: 595.97

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

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:

Sutlu *et al* (2012) Inhibition of intracellular antiviral defense mechanisms augments lentiviral transduction of human natural killer cells: implications for gene therapy. *Hum. Gene Ther.* **23** 1090. PMID: 22779406.

Clark *et al* (2009) Use of the pharmacological inhibitor BX795 to study the regulation and physiological roles of TBK1 and IκB kinase ε: a distinct upstream kinase mediates Ser-172 phosphorylation and activates J.Biol.Chem. **284** 14136. PMID: 19307177.

Tamguney *et al* (2008) Analysis of 3-phosphoinositide-dependent kinase-1 signaling and function in ES cells. *Exp.Cell Res.* **314** 2299. PMID: 18514190.

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