

# Certificate of Analysis

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**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:** C<sub>23</sub>H<sub>26</sub>IN<sub>7</sub>O<sub>2</sub>S.¼H<sub>2</sub>O

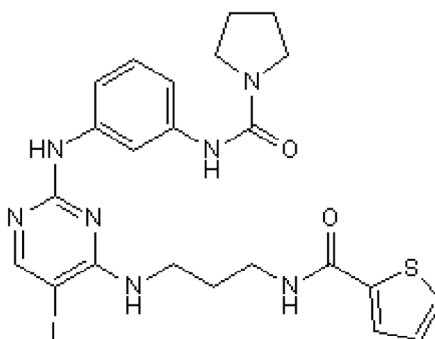
**Batch Molecular Weight:** 595.97

**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<sub>f</sub> = 0.63 (Ethyl acetate)

**HPLC:** Shows 98.8% purity

**<sup>1</sup>H 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:**

BX 795 is an 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:**

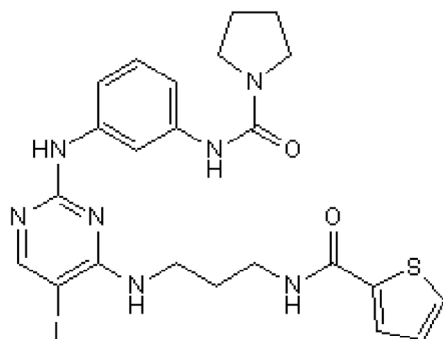
Batch Molecular Formula: C<sub>23</sub>H<sub>26</sub>IN<sub>7</sub>O<sub>2</sub>S.½H<sub>2</sub>O

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. \*Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

**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 activation. *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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