

**Product Name:** BX 795

**Catalog No.:** 4318

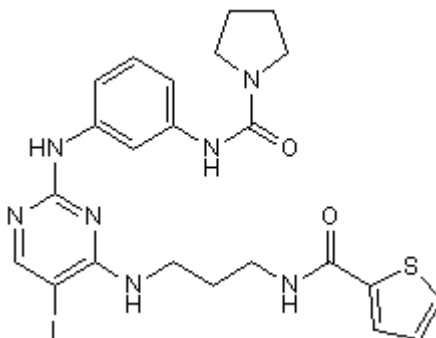
**Batch No.:** 1

**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.2½H<sub>2</sub>O  
**Batch Molecular Weight:** 636.51  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
 ethanol to 100 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows 98% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	43.4	4.91	15.4
Found	43.16	4.77	15.48

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 (PDK1). 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).

**Physical and Chemical Properties:**

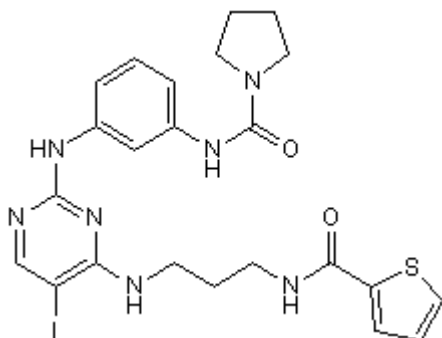
Batch Molecular Formula: C<sub>23</sub>H<sub>26</sub>N<sub>7</sub>O<sub>2</sub>S.2½H<sub>2</sub>O

Batch Molecular Weight: 636.51

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:**

**Feldman et al** (2005) Novel small molecule inhibitors of 3-phosphoinositide-dependent kinase-1. *J.Biol.Chem.* **280** 19867. PMID: 15772071.

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

**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.

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