

Product Data Sheet

Product Name: BX795
Cat. No.: GC11573

Chemical Properties

Cas. No. 702675-74-9

Chemical Name N-[3-[[5-iodo-4-[3-(thiophene-2-carbonylamino)propylamino]pyrimidin-2-yl]amino]phenyl]pyrrolidine-1-carboxamide

SMILES C1CCN(C1)C(=O)NC2=CC=CC(=C2)NC3=NC=C(C(=N3)NCCCNC(=O)C4=CC=CS4)I

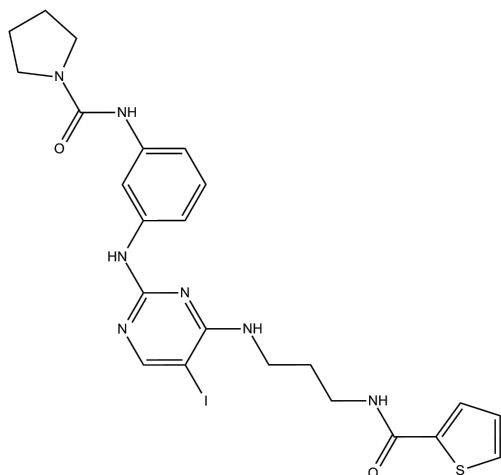
Formula $C_{23}H_{26}IN_7O_2S$ M.Wt 591.48

Solubility ≥ 59.1 mg/mL in DMSO with gentle warming Storage Store at -20°C

General tips For obtaining a higher solubility, please warm the tube at 37°C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice. All other available size: ship with RT, or blue ice upon request.

Structure



Protocol

Cell experiment [1]:

Caution: Product has not been fully validated for medical applications. For research use only.

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Cell lines PC-3 cells

Preparation Method PC-3 cells were treated with BX795 for 18h and analyzed its effects on a number of PDK1 targets using Western blotting.

Reaction Conditions 0.1-10 μ M; 18h

Applications BX795 dose-dependently inhibited the levels of phospho-Thr308-Akt and phospho-Thr389-S6K1.

Animal experiment [2]:

Animal models Brain metastatic mouse model (BCBM)

Preparation Method Developed a brain metastatic mouse model by intracarotid injection of MDA-MB-231-Br cells into the nude mice. Mice were treated with or without TBK1 inhibitor BX795 (20mg/kg; i.p.; every other day for 8 doses) beginning at day 8 post-intracranial injection.

Dosage form 20mg/kg; i.p.; every other day for 8 doses

Applications BX795 significantly reduced brain metastasis and extended survival. BX795 treatment reduced metastatic outgrowth in the brain.

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References:[1] Feldman RI, Wu JM, Polokoff MA, et al. Novel small molecule inhibitors of 3-phosphoinositide-dependent kinase-1. J Biol Chem. 2005;280(20):19867-19874. doi:10.1074/jbc.M501367200. [2] Khan F, Petrosyan E, Liu Y, et al. Microglial TBK1 Signaling Promotes Breast Cancer Brain Metastasis. Cancer Res. 2026;86(1):12-21.

Background

BX795 is an inhibitor of 3-phosphoinositide-dependent protein kinase 1 (PDK1), with an IC₅₀ value of 11nM. BX795 blocks the PDK1/Akt signaling pathway in tumor cells, inhibits the anchorage-dependent growth of various tumor cell lines in vitro, or induces their apoptosis. BX795 also inhibits TANK-binding kinase 1 (TBK1) and IκB kinase ε (IKKε), with the IC₅₀ values of 6 and 41nM, respectively. BX795 potently inhibits diverse HSV-1 strains across transformed human cells, primary corneal cultures (human and animal), and murine ocular surface models. BX795 shows substantial promise as a broad-spectrum human antiviral^{[1][2][3]}.

In vitro, BX795 (0.1-10μM; 18h) dose-dependently inhibited the levels of phospho-Thr308-Akt and phospho-Thr389-S6K1 in PC-3 cells^[1]. BX795 potently inhibited the growth of PC-3 cells in soft agar, displaying IC₅₀ value of 0.25μM^[1]. BX795 (1μM; 60min) blocks TBK1- and IKKε-mediated Activation of IRF3 and Production of IFN-β in HEK293-TLR3 cells^[2]. BX795 (3.125-25μM; 24h) inhibited the replication of HSV-1 (HF) and HSV-2 (G) in HEC-1-A and Vero cells in a dose-dependent manner^[3].

In vivo, BX795 (20mg/kg; i.p.; every other day for 8 doses) significantly reduced brain metastasis and prolonged survival in brain-metastatic mouse models^[4]. BX795 (0.0473mg/kg; 10μL; twice a week for 8 weeks) alleviated cartilage degeneration, synovitis, and OA pain, and improved cartilage inflammation, senescence, and matrix metabolism in Destabilization of the Medial Meniscus (DMM)-induced mouse osteoarthritis models^[5].

References:

[1] Feldman RI, Wu JM, Polokoff MA, et al. Novel small molecule inhibitors of 3-phosphoinositide-dependent kinase-1. J Biol Chem. 2005;280(20):19867-19874. doi:10.1074/jbc.M501367200.

[2] Clark K, Plater L, Pegg M, Cohen P. Use of the pharmacological inhibitor BX795 to study the

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regulation and physiological roles of TBK1 and I κ B kinase epsilon: a distinct upstream kinase mediates Ser-172 phosphorylation and activation. J Biol Chem. 2009;284(21):14136-14146.

[3] Su AR, Qiu M, Li YL, et al. BX-795 inhibits HSV-1 and HSV-2 replication by blocking the JNK/p38 pathways without interfering with PDK1 activity in host cells. Acta Pharmacol Sin. 2017;38(3):402-414.

[4] Khan F, Petrosyan E, Liu Y, et al. Microglial TBK1 Signaling Promotes Breast Cancer Brain Metastasis. Cancer Res. 2026;86(1):12-21.

[5] Lu R, Qu Y, Wang Z, et al. TBK1 pharmacological inhibition mitigates osteoarthritis through attenuating inflammation and cellular senescence in chondrocytes. J Orthop Translat. 2024;47:207-222.

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