BS-181 hydrochloride

Cat. No.: HY-13266A

CAS No.: 1397219-81-6

Molecular Formula: $C_{22}H_{33}ClN_6$

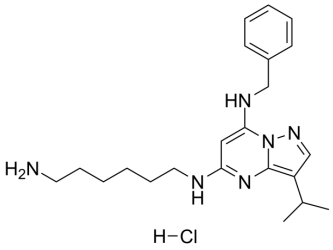
Molecular Weight: 417

Target: CDK

Pathway: Cell Cycle/DNA Damage

Storage: 4°C, sealed storage, away from moisture

* In solvent : -80°C, 2 years; -20°C, 1 year (sealed storage, away from moisture)



SOLVENT & SOLUBILITY

In Vitro

H_2O : 100 mg/mL (239.81 mM; Need ultrasonic)

DMSO : ≥ 50 mg/mL (119.90 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.3981 mL	11.9904 mL	23.9808 mL
5 mM	0.4796 mL	2.3981 mL	4.7962 mL
10 mM	0.2398 mL	1.1990 mL	2.3981 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: PBS
   Solubility: 50 mg/mL (119.90 mM); Clear solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 3 mg/mL (7.19 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 3 mg/mL (7.19 mM); Clear solution
4. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 3 mg/mL (7.19 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

BS-181 hydrochloride is a highly selective CDK7 inhibitor with IC_{50} of 21 nM, and > 40-fold selective for CDK7 than CDK1, 2, 4, 5, 6, or 9.

IC_{50} & Target

CDK7/CycH/MAT1	CDK2/Cyc E	CDK5/p35NCK	CDK9/cycT
0.021 μM (IC_{50})	0.88 μM (IC_{50})	3 μM (IC_{50})	4.2 μM (IC_{50})

	CDK1/cycB 8.1 μM (IC_{50})	CDK4/Cyc D1 33 μM (IC_{50})	CDK6/cycD1 47 μM (IC_{50})
In Vitro	BS-181 promotes cell cycle arrest and inhibits cancer cell growth, and growth is inhibited for all cell lines tested, with IC_{50} values ranging from 11.5 to 37 μM. BS-181 inhibits RB phosphorylation at Ser^{795} and Ser^{821} with an apparent IC_{50} of 15 μM, similar to the IC_{50} obtained for P-Ser2 inhibition. BS-181 treatment of MCF-7 cells leads to G1 arrest at and apoptosis[1]. BS-181 inhibits GC cell and normal gastric epithelial RGM-1 cell line growth with inhibitory concentration (IC_{50}) ranging from 17 to 22 μM and 6.5 μM, respectively. BS-181 significantly inhibits cell migration and invasion ability in a dose-dependent manner[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.		
In Vivo	BS-181 (5 mg/kg, 10 mg/kg, i.p.) inhibits the growth of MCF-7 tumors in nude mice. Intravenous (i.v) and i.p administration of 10 mg/kg BS-181 shows rapid clearance[1]. BS-181 (10 mg/kg/d or 20 mg/kg/d, i.p.) significantly inhibits the growth of tumor in a dose-dependent manner compared to the control group[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.		

PROTOCOL

Cell Assay [2]	Cell viability is detected using Cell Counting Kit (CCK-8 kit) according to supplier's introductions. Briefly, BGC823 cells are seeded at 10^4 cells per well for 48 hours with or without BS-181. Then, the absorbance is detected at 450 nm (reference at 650 nm) in each well. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
Animal Administration [2]	In total, 5×10^6 BGC823 cells (0.1 mL) are injected subcutaneously into the flank of the mice. Tumor measurements are performed two times per week, and volumes are calculated using the formula: tumor size=(length ×$width^2$)/2. Finally, 30 mice (tumor volume 100-200 mm^3) are selected and randomLy assigned into three groups. As previously described, BS-181 is prepared in 10% dimethyl sulfoxide/50 mM HCl/5% Tween 20/85% saline. Micereceive BS-181 injection (ip) twice daily at indicated doses (BS-181 [10 mg/kg/d or 20 mg/kg/d] or Roscovitine [20 mg/kg/d]) for a total of 14 days. Control mice are injected with vehicles. Animal weights and tumor volume are measured each day throughout the 14-day treatment. In addition, all rats are kept for another 30 days for survival observation. Mice are injected intraperitoneally twice daily with BS-181 at 5 mg/kg or 10 mg/kg. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Theranostics. 2017 Apr 20;7(7):1914-1927.
- Cell Rep. 2017 Dec 5;21(10):2796-2812.
- Biochem Biophys Res Commun. 2019 Jun 11;513(4):967-973.

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REFERENCES

[1]. Ali S et al. The development of a selective cyclin-dependent kinase inhibitor that shows antitumor activity. Cancer Res. 2009 Aug 1;69(15):6208-15.

[2]. Wang BY, et al. Selective CDK7 inhibition with BS-181 suppresses cell proliferation and induces cell cycle arrest and apoptosis in gastric cancer. Drug Des Devel Ther. 2016 Mar 16;10:1181-9.

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

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