# BS-181 hydrochloride

**Cat. No.:** HY-13266A

**CAS No.:** 1397219-81-6

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

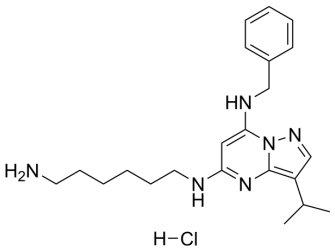
**Molecular Weight:** 416.99

**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 (119.91 mM)

* "≥" means soluble, but saturation unknown.

**Preparing Stock Solutions**

| Solvent / Mass / Concentration | 1 mg | 5 mg | 10 mg |
|---|---|---|---|
| 1 mM | 2.3981 mL | 11.9907 mL | 23.9814 mL |
| 5 mM | 0.4796 mL | 2.3981 mL | 4.7963 mL |
| 10 mM | 0.2398 mL | 1.1991 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 (119.91 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<br>8.1 μM ($IC_{50}$) | CDK4/Cyc D1<br>33 μM ($IC_{50}$) | CDK6/cycD1<br>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].<br>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].<br>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.<br>MCE has not independently confirmed the accuracy of these methods. They are for reference only. |
| **Animal Administration** [2] | In total, $5\times10^6$ 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.<br>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.
- Universidade de Lisboa. 2021 Dec 21.

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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.



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