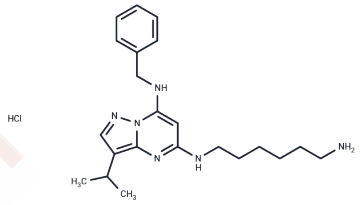
Data Sheet (Cat.No.T6162)

TargetMol

BS-181 hydrochloride

Chemical Properties



CAS No. : 1397219-81-6

Formula: C22H32N6·HCl

Molecular Weight: 416.99

Appearance: no data available

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Biological Description

Description	BS-181 hydrochloride (BS-181 HCl) is a highly selective CDK7 inhibitor with IC50 of 21 nM. It is more than 40-fold selective for CDK7 than CDK1, 2, 4, 5, 6, or 9.
Targets(IC50)	CDK
In vitro	BS-181 is a small molecule inhibitor of CDK7 in a cell-free environment, which displays more potential activity than roscovitine with IC 50 of 510 nM. Among the CDKs and other 69 kinases from many different classes, BS-181 shows high inhibitory selectivity for CDK7, inhibits CDK2 at concentrations lower than 1 μM which being inhibited 35-fold less potently (IC50 with 880 nM) than CDK7, shows slight inhibition for CDK1, CDK4, CDK5, CDK6 and CDK9 with IC50 values higher than 3.0 μM, and only shows inhibition for several kinases from other classes at high concentrations (>10 μM). BS-181 promotes cell cycle arrest and inhibits the cancer cell growth of a range of tumor types, including breast, lung, prostate and colorectal cancer with IC50 in the range of 11.5-37 μM. In MCF-7 cells, BS-181 inhibits the phosphorylation of the CDK7 substrate RNA polymerase II COOH-terminal domain (CTD), and promotes cell cycle arrest and apoptosis to inhibit the growth of cancer cell lines. [1]
In vivo	BS-181 is stable in vivo with a plasma elimination half-life in mice of 405 minutes after i. p. administration of 10 mg/kg. BS-181 inhibits the growth of MCF-7 xenografts in the nude mice model in a dose-dependent manner, with 25% and 50% reduction in tumor growth after 2 weeks of treatment at 10 mg/kg/day and 20 mg/kg/day, respectively without apparent toxicity. [1]
Kinase Assay	In vitro kinase inhibition.: Inhibition of CDK7 activity is measured by incubation of increasing amounts of BS-181 with purified recombinant CDK7/CycH/MAT1 complex, followed by measurement of free ATP remaining in the reaction using a luciferase assay, luciferase activity therefore providing a measure of inhibition of CDK7 activity for the determination of IC50.
Cell Research	MCF-7 cells are exposed to BS-181 for 24 hours. For the determination of cell cycle and apoptosis, cells are stained with propidium iodide or labeled with Annexin V-FITC, then labeled cells are acquired within 1 hour, by using the RXP cytomics software on a Beckman Coulter Elite ESP, and the data are analyzed using Flow Jo v7.2.5. For the assessment of CDKs, cells are lysed and analyzed by western blotting.(Only for Reference)

Solubility Information

Solubility	Ethanol: 22 mg/mL (52.75 mM),Heating is recommended. H2O: 50 mg/mL (119.9 mM),Sonication is recommended. DMSO: 100 mg/mL (239.8 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
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
50 mM	0.048 mL	0.2398 mL	0.4796 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Reference

Ali S, et al. Cancer Res, 2009, 69(15), 6208-6215.