Screening Libraries

Product Data Sheet

Bohemine

Cat. No.: HY-12843 CAS No.: 189232-42-6 Molecular Formula: $C_{18}H_{24}N_{6}O$ Molecular Weight: 340.42 Target: CDK; ERK

Pathway: Cell Cycle/DNA Damage; MAPK/ERK Pathway; Stem Cell/Wnt

Storage: Powder -20°C 3 years In solvent -80°C 6 months

> -20°C 1 month

SOLVENT & SOLUBILITY

In Vitro

DMSO: 100 mg/mL (293.75 mM; Need ultrasonic)

	Solvent Mass Concentration	1 mg	5 mg	10 mg
Preparing Stock Solutions	1 mM	2.9375 mL	14.6877 mL	29.3755 mL
	5 mM	0.5875 mL	2.9375 mL	5.8751 mL
	10 mM	0.2938 mL	1.4688 mL	2.9375 mL

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

In Vivo

- 1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 2.5 mg/mL (7.34 mM); Clear solution
- 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.5 mg/mL (7.34 mM); Clear solution
- 3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.5 mg/mL (7.34 mM); Clear solution

BIOLOGICAL ACTIVITY

Description Bohemine is a purine analogue and is a synthetic and selective CDK inhibitor with IC₅₀s of 4.6 μM, 83 μM, and 2.7 μM for $Cdk2/cyclin\ E,\ Cdk2/cyclin\ A,\ and\ Cdk9/cyclin\ T1,\ respectively.\ Bohemine\ also\ inhibits\ ERK2\ with\ an\ IC_{50}\ of\ 52\ \mu M\ and\ has\ New And\ New And\$ less inhibitory effect on CDK1, CDK4 and CDK6. Bohemine has a broad spectrum anti-cancer activities^{[1][2]}.

IC₅₀ & Target CDK2/cyclinE cdk2/cyclin A CDK9/cyclinT1 ERK2 $2.7 \, \mu M \, (IC_{50})$ $4.6 \, \mu M \, (IC_{50})$ 83 μM (IC₅₀) 52 μM (IC₅₀)

In Vitro Bohemine (0-30 μM; 72 hours; ME-750 cells) treatment inhibits cell growth. Addition of Bohemine at concentrations in the range of 1-10 μ M results in a short-term arrest of growth and of monoclonal antibody production. The short-term suppression of cell functions is followed by a significant temporary increase of specific growth rate and of specific production rate^[1].

Hybridoma cells are retarded both at the G1/S boundary and at the G2/M boundary, depending on Bohemine (0-30 μ M) concentration^[1].

T-lymphoblastic cell line CEM is treated by Bohemine, five proteins are found to be downregulated, namely α -enolase, triosephosphate isomerase, initiation factor 5A, and α - and β -subunits of Rho GDP-dissociation inhibitor 1. These proteins play significant roles in glycolysis, proteosynthesis, and in cytoskeleton rearrangement^[1].

Bohemine inhibits growth of human tumor cell lines with an IC₅₀ of 27 μ M^[2].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Viability Assay^[1]

Cell Line:	Mouse hybridoma ME-750 cells	
Concentration:	0 μ M, 1 μ M, 3 μ M, 10 μ M and 30 μ M	
Incubation Time:	72 hours	
Result:	At 10 μM and 30 μM concentrations, the viable cell count was significantly lower with respect to control, i.e., 77% and 48%, respectively.	

In Vivo

Bohemine (50 mg/kg; intravenous injection; BALB/c mice) treatment shows C_{max} is 72,308 nM, observed clearance is 0.23 L/h and $T_{1/2}$ is 1.39 h^[2].

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Animal Model:	BALB/c mice bearing the colon 26 murine tumor ^[2]	
Dosage:	50 mg/kg	
Administration:	Intravenous injection (Pharmacokinetic Analysis)	
Result:	$\rm C_{max}$ is 72,308 nM, observed clearance is 0.23 L/h and $\rm T_{1/2}$ is 1.39 h.	

CUSTOMER VALIDATION

• EMBO Rep. 2022 Apr 11;e53932.

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REFERENCES

[1]. Franek F, et al. Diverse effects of the cyclin-dependent kinase inhibitor bohemine: Concentration- and time-dependent suppression or stimulation of hybridoma culture. Cytotechnology. 2001 Jul;36(1-3):117-23.

[2]. Raynaud FI, et al. In vitro and in vivo pharmacokinetic-pharmacodynamic relationships for the trisubstituted aminopurine cyclin-dependent kinase inhibitors olomoucine, bohemine and CYC202. Clin Cancer Res. 2005 Jul 1;11(13):4875-87.

 $\label{lem:caution:Product} \textbf{Caution: Product has not been fully validated for medical applications. For research use only.}$

Tel: 609-228-6898 Fax: 609-228-5909

E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA

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