BPH-1358

Cat. No.: HY-118946

CAS No.: 5352-53-4

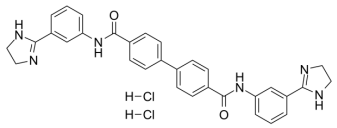
Molecular Formula: $C_{32}H_{30}Cl_2N_6O_2$

Molecular Weight: 601.53

Target: Bacterial

Pathway: Anti-infection

Storage: 4°C, protect from light
* In solvent : -80°C, 6 months; -20°C, 1 month (protect from light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 6.25 mg/mL (10.39 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.6624 mL	8.3121 mL	16.6243 mL
	5 mM	0.3325 mL	1.6624 mL	3.3249 mL
	10 mM	0.1662 mL	0.8312 mL	1.6624 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 0.62 mg/mL (1.03 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 0.62 mg/mL (1.03 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

BPH-1358 (NSC50460) is a potent human farnesyl diphosphate synthase (FPPS) and undecaprenyl diphosphate synthase (UPPS) inhibitor with IC_{50}s of 1.8 μM and 110 nM, respectively, and is active against ***S. aureus*** in vitro (MIC ~250 ng/mL)[1][2].

IC_{50} & Target

IC50: 1.8 μM (human bisphosphonate farnesyl diphosphate synthase)[1]; 100 nM (undecaprenyl diphosphate synthase)[2]

In Vitro

BPH-1358 is the most potent inhibitor of both E. coli UPPS (EcUPPS) as well as S. aureus UPPS (SaUPPS) with an IC_{50} of 110 nM. BPH-1358 against E. coli and S. aureus with EC_{50} of 300 nM and 290 nM, respectively[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

BPH-1358 is active against S. aureus in vivo (20/20 mice survived in an i.p. infection model with a MRSA strain)[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Liu YL, et al. Farnesyl diphosphate synthase inhibitors with unique ligand-binding geometries. ACS Med Chem Lett. 2015 Jan 29;6(3):349-54.

[2]. Zhu W, et al. Antibacterial drug leads: DNA and enzyme multitargeting. J Med Chem. 2015 Feb 12;58(3):1215-27.

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