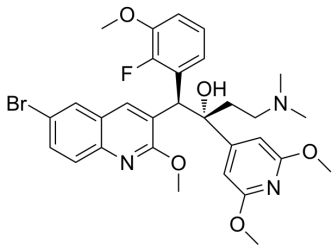
TBAJ-587

Cat. No.:	HY-111747
CAS No.:	2252316-16-6
Molecular Formula:	$C_{30}H_{33}BrFN_3O_5$
Molecular Weight:	614.5
Target:	Bacterial
Pathway:	Anti-infection
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 2 years -20°C 1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 43.33 mg/mL (70.51 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.6273 mL	8.1367 mL	16.2734 mL
	5 mM	0.3255 mL	1.6273 mL	3.2547 mL
	10 mM	0.1627 mL	0.8137 mL	1.6273 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: ≥ 2.17 mg/mL (3.53 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.17 mg/mL (3.53 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.17 mg/mL (3.53 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

TBAJ-587, a potent anti-tuberculosis agent, inhibits M.tb strain H37Rv growth with MIC_{90}s of 0.006 and <0.02 μg/mL in MABA and LORA assay, respectively. TBAJ-587 inhibits hERG channel minimally, attenuates inhibition of the cardiac potassium channel protein coded by the hERG, which is important for cardiac repolarization[1].

IC_{50} & Target

Anti-tuberculosis[1]

In Vitro

Bedaquiline is a drug of the diarylquinoline class that has proven to be clinically effective against drug-resistant

tuberculosis, but has a cardiac liability due to its potent inhibition of the cardiac potassium channel protein hERG. TBAJ-587, an analogue of Bedaquiline, demonstrates more potent anti-tubercular activity, with greatly attenuated hERG blockade. TBAJ-587 inhibits hERG channel with an IC_{50} of 13 μM[1].

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

REFERENCES

[1]. Sutherland HS, et al. 3,5-Dialkoxypyridine analogues of bedaquiline are potent antituberculosis agents with minimal inhibition of the hERG channel. Bioorg Med Chem. 2019 Apr 1;27(7):1292-1307.

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