Bedaquiline

Cat. No.: HY-14881

CAS No.: 843663-66-1

Molecular Formula: $C_{32}H_{31}BrN_2O_2$

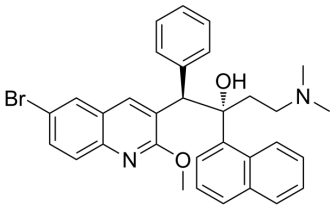
Molecular Weight: 555.5

Target: Bacterial; Antibiotic

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 : 12.5 mg/mL (22.50 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	1.8002 mL	9.0009 mL	18.0018 mL
	5 mM	0.3600 mL	1.8002 mL	3.6004 mL
	10 mM	0.1800 mL	0.9001 mL	1.8002 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: ≥ 0.5 mg/mL (0.90 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 0.5 mg/mL (0.90 mM); Suspended solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 0.5 mg/mL (0.90 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Bedaquiline (TMC207) is a diarylquinoline agent and inhibits Mycobacterium tuberculosis (Mtb) F1FO-ATP synthase through targeting of both the c- and the ε-subunit[1]. Bedaquiline has uncoupler activity. Bedaquiline is used for the multi-agent resistant tuberculosis[2].

IC_{50} & Target

Mtb F1FO-ATP synthase[1]

In Vitro

Bedaquiline inhibits the growth of TDR M. tuberculosis strains, with MIC values ranging from 0.125 to 0.5 mg/L[2].

Among slowly growing mycobacteria (SGM), bedaquiline exhibits the highest activity against Mycobacterium avium with MIC_{50} and MIC_{90} values of 0.03 and 16 mg/L, respectively. Among rapidly growing mycobacteria (RGM), Mycobacterium abscessus subsp. abscessus (M. abscessus) and Mycobacterium abscessus subsp. massiliense (M. massiliense) seem more susceptible to bedaquiline than Mycobacterium fortuitum, with MIC_{50} and MIC_{90} values of 0.13 and >16 mg/L, respectively, for both species. Bedaquiline also shows moderate in vitro activity against NTM species[3].
Bedaquiline has an excellent in vitro activity against Mycobacterium tuberculosis, including multidrug resistant M tuberculosis[4].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Cell. 2023 May 11;186(10):2176-2192.e22.
- Nat Commun. 2021 Jun 21;12(1):3816.
- Eur J Med Chem. 6 August 2022, 114639.
- Mbio. 2021 Jun 1;e0108821.
- Front Cell Infect Microbiol. 2016 Nov 8;6:145. eCollection 2016.

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REFERENCES

[1]. Jang JC, et al. Bedaquiline susceptibility test for totally drug-resistant tuberculosis Mycobacterium tuberculosis. J Microbiol. 2017 Apr 20.

[2]. Pang Y, et al. In Vitro Activity of Bedaquiline against Nontuberculous Mycobacteria in China. Antimicrob Agents Chemother. 2017 Apr 24;61(5).

[3]. Chahine EB, et al. Bedaquiline: a novel diarylquinoline for multidrug-resistant tuberculosis. Ann Pharmacother. 2014 Jan;48(1):107-15.

[4]. Sarathy JP, et al. TBAJ-876 displays Bedaquiline-like mycobactericidal potency without retaining the parental drug's uncoupler activity. Antimicrob Agents Chemother. 2019 Nov 11.

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