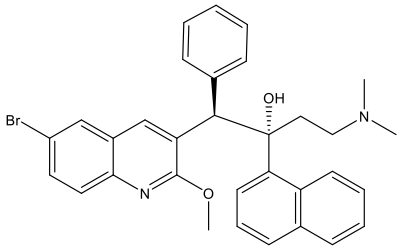
Catalog # 10-4403

Bedaquiline

CAS# 843663-66-1

(1R,2S)-1-(6-Bromo-2-methoxyquinolin-3-yl)-4-(dimethylamino)-2-naphthalen-1-yl-1-phenylbutan-2-ol; TMC207; R207910

Lot # FBS2130



Bedaquiline is a clinically useful antituberculosis agent that is active (MIC's 0.030 to 0.120 µg/mL) against multi-drug resistant strains.[1] It interferes with mycobacterial energy metabolism *via* binding to the oligomeric subunit c (AtpE)[2] and subunit ε[3] of ATP synthase inhibiting ATP production.[4] Bedaquiline has recently been found to be an inhibitor (IC_{50} = 18.7 µM) of the SARS-CoV-2 main protease, 3CLpro.[5]

1) Andries *et al.* (2005), *A diarylquinoline drug active on the ATP synthase of Mycobacterium tuberculosis*; Science, **307** 223
2) Koul *et al.* (2007), *Diarylquinolines target subunit c of mycobacterial ATP synthase*; Nat. Chem. Biol., **3** 323
3) Biukovic *et al.* (2013), *Variations of subunit {varepsilon} of the Mycobacterium tuberculosis F1F0 ATP synthase and a novel model for mechanism of action of the tuberculosis drug TMC207*; Antimicrob. Agents Chemother., **57** 168
4) Sarathy *et al.* (2019), *Re-Understanding the Mechanisms of Action of the Anti-Mycobacterial Drug Bedaquiline*; Antibiotics (Basel), **8** 261
5) Ghahremanpour *et al*. (2020), *Identification of 14 Known Drugs as Inhibitors of the Main Protease of SARS-CoV-2*; ACS Med. Chem. Lett., **11** 2526

PHYSICAL DATA

Molecular Weight:	555.50
Molecular Formula:	$C_{32}H_{31}BrN_2O_2$
Purity:	99% by HPLC
	NMR: (Conforms)
Solubility:	DMSO (10 mg/ml)
Physical Description:	White solid
Storage and Stability:	Store as supplied at room temperature for up to 1 year from the date of purchase. Solutions in DMSO may be stored at -20°C for up to 1 month.

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