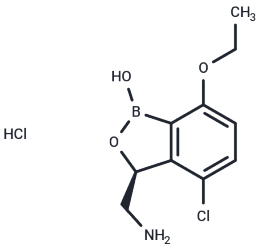
Data Sheet (Cat.No.T38773)

TargetMol
YOUR TARGET MOLECULES

LeuRS-IN-1 hydrochloride

Chemical Properties



CAS No. : 1364683-67-9

Formula: C10H14BCl2NO3

Molecular Weight: 277.94

Appearance: no data available

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Biological Description

Description	LeuRS-IN-1 hydrochloride is a potent and orally active inhibitor of M. tuberculosis leucyl-tRNA synthetase (M.tb LeuRS). It has IC 50 and Kd values of 0.06 μM and 0.075 μM, respectively, for M.tb LeuRS. Additionally, LeuRS-IN-1 hydrochloride inhibits human cytoplasmic LeuRS with an IC 50 of 38.8 μM and HepG2 protein synthesis with an EC 50 of 19.6 μM.
In vitro	LeuRS-IN-1 (compound 13) hydrochloride exhibits potent antibacterial activity against M.tb H37Rv, showcasing a minimum inhibitory concentration (MIC) value of 0.02 μg/mL[1]. Additionally, LeuRS-IN-1 (compound 3a) hydrochloride demonstrates cytotoxic effects on HepG2 cells after 48 hours of exposure, with an effective concentration (EC 50) value of 65.8 μM[2].
In vivo	LeuRS-IN-1 hydrochloride, administered orally at a dosage of 100 mg/kg daily for 14 days, effectively reduces lung colony-forming unit (CFU) values in mice with acute tuberculosis (TB) [1]. A lower dosage of 33 mg/kg, administered orally five days a week for four weeks, significantly decreases lung and spleen CFU values in mice with chronic TB [1]. Pharmacokinetic studies in mice reveal that, following intravenous (i.v.) administration at 30 mg/kg, LeuRS-IN-1 exhibits a maximum concentration (C max) of 13.6 μg/ml at 5 minutes, a clearance (CL) of 582 ml/h/kg, a steady-state volume of distribution (V ss) of 3,142 ml/kg, a mean residence time (MRT) of 5.4 hours, an area under the curve (AUC) 0-∞ of 51.6 h · μg/ml, an alpha half-life (α-t 1/2) of 0.10 hours (2% AUC), and a beta half-life (β-t 1/2) of 3.83 hours (98% AUC). Oral administration (p.o.) at the same dose achieves a C max of 6.4 μg/ml at 0.25 hours, an AUC 0-24 of 47.5 h · μg/ml, a terminal half-life of 3.1 hours, and a bioavailability of 9.2%. In murine GKO (C57BL/6-Ifngtm1ts) model of acute TB, 100 mg/kg of LeuRS-IN-1, given orally daily for 14 days post-infection with M. tuberculosis Erdman, reduces lung CFU counts. Similarly, in the BALB/c model of chronic TB infection, 33 mg/kg administered orally five days a week for four weeks, starting 21 days post-low-dose aerosol infection with M. tuberculosis Erdman, leads to decreased lung and spleen CFU counts [1].

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	3.5979 mL	17.9895 mL	35.979 mL
5 mM	0.7196 mL	3.5979 mL	7.1958 mL
10 mM	0.3598 mL	1.7989 mL	3.5979 mL
50 mM	0.072 mL	0.3598 mL	0.7196 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Reference

Palencia A, et al. Discovery of Novel Oral Protein Synthesis Inhibitors of Mycobacterium tuberculosis That Target Leucyl-tRNA Synthetase. Antimicrob Agents Chemother . 2016;60(10):6271-6280. Published 2016 Sep 23.