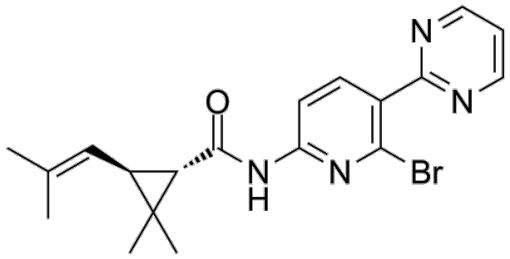
Product Data Sheet

Product Name: BRD-8000.3
Cat. No.: GC62876

Chemical Properties

Cas. No.	2365504-95-4		
Formula	$C_{19}H_{21}BrN_4O$	M.Wt	401.3
Solubility	DMSO : 50 mg/mL (124.60 mM; Need ultrasonic)	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 °C and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20°C for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		

Structure



Protocol

Animal experiment [1]:

Product Data Sheet

Animal models	C57BL/6 mice
Preparation Method	Oral dosing of 12h fasted female 7-9-week-old C57BL/6 mice was performed, using 150mg/kg BRD-8000.3 in 5% (v/v) corn oil, 10% (v/v) labrasol, 5% (v/v) solutol in water. The plasma concentration of BRD-8000.3 was measured at nine time points up to 8h.
Dosage form	150mg/kg; p.o.
Applications	BRD-8000.3 showed good mouse plasma exposure by oral dosing. The half-life of BRD-8000.3 in mice is 5min.

References:
[1] Johnson EO, LaVerriere E, Office E, et al. Large-scale chemical-genetics yields new M. tuberculosis inhibitor classes. *Nature*. 2019;571(7763):72-78.

Background

BRD-8000.3, as a specific EfpA inhibitor, is a narrow-spectrum, bactericidal antimycobacterial agent with good wild-type activity[1]. BRD-8000.3 exhibits inhibitory activity against Mycobacterium tuberculosis (Mtb) with an MIC_{90} value of 800nM[1]. Resistance to BRD-8000.3 could be conferred by mutations in EfpA, including substitutions V319F and A415V[2].

In vitro, BRD-8000.3 has an IC_{50} value greater than 50μM for HepG2[3].

In vivo, BRD-8000.3, administered orally at 150mg/kg, demonstrated good mouse plasma exposure and low risk for drug–drug interactions, prolongation of the QT interval, or hepatotoxicity[3].

References:
[1] Johnson EO, et al. Large-Scale Chemical-Genetic Strategy Enables the Design of Antimicrobial Combination Chemotherapy in Mycobacteria. ACS Infect Dis. 2020;6(1):56-63.
[2] Khandelwal NK, Gupta M, Gomez JE, et al. Structure and inhibition mechanisms of *Mycobacterium tuberculosis* essential transporter efflux protein A. Preprint. *bioRxiv*.

Caution: Product has not been fully validated for medical applications. For research use only.
Tel: (909) 407-4943 Fax: (626) 353-8530 E-mail: tech@glpbio.com
Address: 10292 Central Ave. #205, Montclair, CA, USA

Product Data Sheet

2024;2024.09.04.611325.
[3] Johnson EO, LaVerriere E, Office E, et al. Large-scale chemical-genetics yields new M. tuberculosis inhibitor classes. *Nature*. 2019;571(7763):72-78.

Caution: Product has not been fully validated for medical applications. For research use only.
Tel: (909) 407-4943 Fax: (626) 353-8530 E-mail: tech@glpbio.com
Address: 10292 Central Ave. #205, Montclair, CA, USA