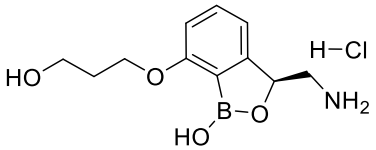
Product data sheet

MedKoo Cat#: 319569 Name: Epetraborole HCl CAS#: 1234563-16-6 (HCl) Chemical Formula: $C_{11}H_{17}BClNO_4$ Molecular Weight: 273.52	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:

Epetraborole, also known as GSK2251052 and AN3365, is a potent and selective leucyl-tRNA synthetase inhibitor. Epetraborole was in development for the treatment of infections caused by multidrug-resistant Gram-negative pathogens. GSK2251052 is a novel boron-containing antibiotic that inhibits bacterial leucyl tRNA synthetase. All Clostridium perfringens strains had GSK2251052 MICs of >32 μg/ml.

2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	200.0	731.21
Water	28.0	102.37

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	**1 mg**	**5 mg**	**10 mg**
1 mM	3.66 mL	18.28 mL	36.56 mL
5 mM	0.73 mL	3.66 mL	7.31 mL
10 mM	0.37 mL	1.83 mL	3.66 mL
50 mM	0.07 mL	0.37 mL	0.73 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study

In vitro study

1. Mendes RE, Alley MR, Sader HS, Biedenbach DJ, Jones RN. Potency and spectrum of activity of AN3365, a novel boron-containing protein synthesis inhibitor, tested against clinical isolates of Enterobacteriaceae and nonfermentative Gram-negative bacilli. Antimicrob Agents Chemother. 2013 Jun;57(6):2849-57. doi: 10.1128/AAC.00160-13. Epub 2013 Mar 18. PMID: 23507283; PMCID: PMC3716140.

In vivo study

1. Kim T, Hanh BT, Heo B, Quang N, Park Y, Shin J, Jeon S, Park JW, Samby K, Jang J. A Screening of the MMV Pandemic Response Box Reveals Epetraborole as a New Potent Inhibitor against Mycobacterium abscessus. Int J Mol Sci. 2021 May 31;22(11):5936. doi: 10.3390/ijms22115936. PMID: 34073006; PMCID: PMC8199016.

7. Bioactivity

Biological target:

Epetraborole hydrochloride is a novel leucyl-tRNA synthetase (LeuRS) inhibitor.

In vitro activity

Product data sheet

AN3365 ($MIC_{50/90}$, 0.5/1 μg/ml) demonstrated potent activity against *Enterobacteriaceae*, inhibiting all isolates at ≤2 μg/ml, except for one *Proteus vulgaris* strain (MIC, 4 μg/ml). Furthermore, the overall MIC distribution of AN3365 remained constant (MIC_{50}, 0.5 μg/ml) across the tested *Enterobacteriaceae* species, groups of organisms, and resistant subsets. However, slightly higher AN3365 MIC results were observed for *P. mirabilis* isolates ($MIC_{50/90}$, 1/1 μg/ml), suggesting that this species may be less susceptible to this compound than other wild-type strains. In addition, KPC-producing *K. pneumoniae* strains also exhibited higher MIC_{50} results (1 μg/ml) than the respective susceptible counterparts.

Reference: Antimicrob Agents Chemother. 2013 Jun; 57(6): 2849–2857. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3716140/

In vivo activity

In vivo efficacy of ETB was also validated in *Danio rerio* (zebrafish; hereafter referred to as ZF) of infection. To determine whether ETB has the ability to treat *Mab* infected ZF as a therapeutic agent. ETB in vivo efficacy was evaluated in ZF after infection with *Mab* subsp. *abscessus* $CIP104536^T$ R variant that express mWasabi green fluorescence (hereafter referred to as *Mab*R-mWasabi) at concentrations of 6.25, 12.5, 25, and 50 μM. As shown in Figure 4A, *Mab*R-mWasabi was disseminated and localized inside of ZF, especially in the head when the DMSO was treated. However, the mWasabi fluorescent signal was significantly reduced in the ETB treated condition. In more detail, a significant mWasabi reduction in the *Mab*R-mWasabi infected ZF head was observed at 25 μM ETB. Furthermore, almost no mWasabi protein signals were detected in the ZF when *Mab*R-mWasabi infected ZF were treated with 25 and 50 μM ETB.

Reference: Int J Mol Sci. 2021 Jun; 22(11): 5936. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC8199016/