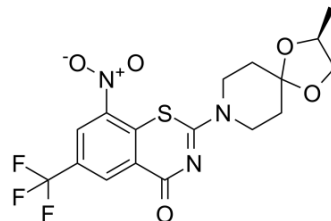


## BTZ043

|                           |  |       |          |
|---------------------------|--|-------|----------|
| <b>Cat. No.:</b>          | HY-13579   |       |          |
| <b>CAS No.:</b>           | 1161233-85-7   |       |          |
| <b>Molecular Formula:</b> | C <sub>17</sub> H <sub>16</sub> F <sub>3</sub> N <sub>3</sub> O <sub>5</sub> S |       |          |
| <b>Molecular Weight:</b>  | 431.39   |       |          |
| <b>Target:</b>            | Bacterial; Antibiotic  |       |          |
| <b>Pathway:</b>           | Anti-infection   |       |          |
| <b>Storage:</b>           | Powder   | -20°C | 3 years  |
|                           |  | 4°C   | 2 years  |
|                           | In solvent   | -80°C | 6 months |
|                           |  | -20°C | 1 month  |



### SOLVENT & SOLUBILITY

|   |  |                          |              |            |            |
|---|--|--------------------------|--------------|------------|------------|
| <b>In Vitro</b>   | DMSO : 13.3 mg/mL (30.83 mM; Need ultrasonic and warming)  |                          |              |            |            |
|   |  | Solvent<br>Concentration | Mass<br>1 mg | 5 mg       | 10 mg      |
|   | <b>Preparing Stock Solutions</b>   | 1 mM                     | 2.3181 mL    | 11.5904 mL | 23.1809 mL |
|   |  | 5 mM                     | 0.4636 mL    | 2.3181 mL  | 4.6362 mL  |
| 10 mM   |  | 0.2318 mL                | 1.1590 mL    | 2.3181 mL  |            |
| Please refer to the solubility information to select the appropriate solvent. |  |                          |              |            |            |
| <b>In Vivo</b>  | <ol style="list-style-type: none"> <li>Add each solvent one by one: 10% DMSO &gt;&gt; 40% PEG300 &gt;&gt; 5% Tween-80 &gt;&gt; 45% saline<br/>Solubility: 2.5 mg/mL (5.80 mM); Suspended solution; Need ultrasonic</li> <li>Add each solvent one by one: 10% DMSO &gt;&gt; 90% (20% SBE-β-CD in saline)<br/>Solubility: 2.5 mg/mL (5.80 mM); Suspended solution; Need ultrasonic</li> <li>Add each solvent one by one: 10% DMSO &gt;&gt; 90% corn oil<br/>Solubility: ≥ 2.5 mg/mL (5.80 mM); Clear solution</li> </ol> |                          |              |            |            |

### BIOLOGICAL ACTIVITY

|                                     |   |
|-------------------------------------|---|
| <b>Description</b>                  | BTZ043 is an inhibitor of decaprenyl-phosphoribose-epimerase (DprE1), with MICs of of 2.3 nM and 9.2 nM for <i>M. tuberculosis</i> H37Rv and <i>Mycobacterium smegmatis</i> , respectively.   |
| <b>IC<sub>50</sub> &amp; Target</b> | DprE1 <sup>[1]</sup> .  |
| <b>In Vitro</b>                     | The MIC of BTZ043 against <i>M. tuberculosis</i> H37Rv and <i>Mycobacterium smegmatis</i> are 1 ng/mL (2.3 nM) and 4 ng/mL (9.2 nM), respectively <sup>[2]</sup> . The in vitro activity of BTZ043 against 30 <i>Nocardia brasiliensis</i> isolates is also tested. The MIC50 and MIC90 |

values for BTZ043 are 0.125 and 0.25 µg/mL. The MIC for *N. carnea* ATCC 6847 is 0.003µg/mL, for *N. transvalensis* ATCC 6865 is 0.003µg/mL, for *N. brasiliensis* NCTC10300 is 0.03 µg/mL, and for *N. brasiliensis* HJJE-1 is 0.125µg/mL. The MIC value for *M. tuberculosis* H37Rv is 0.000976 µg/mL. The MIC value of BTZ-043 is >64 µg/mL for *Escherichia coli* ATCC 25922 and *S. aureus* ATCC 29213<sup>[3]</sup>.

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

#### In Vivo

Four weeks of treatment with BTZ043 reduces the bacterial burden in the lungs and spleens by 1 and 2 logs, respectively, at the concentrations used. Additional results suggest that BTZ043 efficacy is time-rather than dose-dependent. Acute (5 g/kg) and chronic (25 and 250 mg/kg) toxicology studies in uninfected mice show that, even at the highest dose tested, there are no adverse anatomical, behavioral, or physiological effects after one month<sup>[2]</sup>.

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

## PROTOCOL

#### Animal Administration <sup>[2]</sup>

Mice<sup>[2]</sup>

Animal efficacy is determined in a standard mouse infection model. BALB/c mice are infected with a low bacillary load (~200 CFU) of *M. tuberculosis* H37Rv via aerosol. Treatment started four-weeks post infection. Mice are dosed by gavage with 37.5, or 300 mg of BTZ043, per kg body weight, in carboxymethyl cellulose formulation (0.25%), once daily, six times/week, for four weeks. Control and treated mice are sacrificed, lungs and spleens homogenized and dilutions plated for enumeration of viable bacilli<sup>[2]</sup>.

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

## CUSTOMER VALIDATION

- J Med Chem. 2020 May 28;63(10):5367-5386.
- ChemNanoMat. 2020 Oct 28.

See more customer validations on [www.MedChemExpress.com](http://www.MedChemExpress.com)

## REFERENCES

[1]. Vadim Makarov et al. The 8-Pyrrole-Benzothiazinones Are Noncovalent Inhibitors of DprE1 from *Mycobacterium tuberculosis*. *Antimicrob Agents Chemother*, 2015 Aug, 59(8): 4446-4452.

[2]. Makarov V, et al. Benzothiazinones kill *Mycobacterium tuberculosis* by blocking arabinan synthesis. *Science*. 2009 May 8;324(5928):801-4.

[3]. Norma Alejandra González-Martínez et al. In Vivo Activity of the Benzothiazinones PBTZ169 and BTZ043 against *Nocardia brasiliensis*. *PLoS Negl Trop Dis*, 2015 Oct, 9(10): e0004022.

**Caution: Product has not been fully validated for medical applications. For research use only.**

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