



# SZABO SCANDIC

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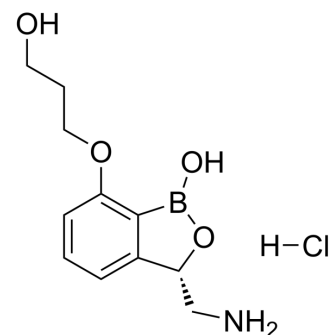
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## Epetraborole hydrochloride

|                    |                                                                                                                                |
|--------------------|--------------------------------------------------------------------------------------------------------------------------------|
| Cat. No.:          | HY-12479A                                                                                                                      |
| CAS No.:           | 1234563-16-6                                                                                                                   |
| Molecular Formula: | C <sub>11</sub> H <sub>17</sub> BClNO <sub>4</sub>                                                                             |
| Molecular Weight:  | 273.52                                                                                                                         |
| Target:            | Bacterial; Aminoacyl-tRNA Synthetase                                                                                           |
| Pathway:           | Anti-infection; Metabolic Enzyme/Protease                                                                                      |
| Storage:           | 4°C, sealed storage, away from moisture<br>* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture) |



### SOLVENT & SOLUBILITY

|                                                                               |                                                                                                                                                                                                                                                                                                                                                                                                                       |                              |                                                      |            |            |       |      |           |            |            |      |           |           |           |       |           |           |           |
|-------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------|------------------------------------------------------|------------|------------|-------|------|-----------|------------|------------|------|-----------|-----------|-----------|-------|-----------|-----------|-----------|
| In Vitro                                                                      | DMSO : 200 mg/mL (731.21 mM; Need ultrasonic)                                                                                                                                                                                                                                                                                                                                                                         |                              |                                                      |            |            |       |      |           |            |            |      |           |           |           |       |           |           |           |
|                                                                               | H <sub>2</sub> O : ≥ 28 mg/mL (102.37 mM)                                                                                                                                                                                                                                                                                                                                                                             |                              |                                                      |            |            |       |      |           |            |            |      |           |           |           |       |           |           |           |
|                                                                               | * "≥" means soluble, but saturation unknown.                                                                                                                                                                                                                                                                                                                                                                          |                              |                                                      |            |            |       |      |           |            |            |      |           |           |           |       |           |           |           |
|                                                                               |                                                                                                                                                                                                                                                                                                                                                                                                                       |                              |                                                      |            |            |       |      |           |            |            |      |           |           |           |       |           |           |           |
|                                                                               |                                                                                                                                                                                                                                                                                                                                                                                                                       |                              |                                                      |            |            |       |      |           |            |            |      |           |           |           |       |           |           |           |
|                                                                               | <table><tr><td rowspan="4">Preparing<br/>Stock Solutions</td><td><div>Solvent<br/>Concentration</div><div>Mass</div></td><td>1 mg</td><td>5 mg</td><td>10 mg</td></tr><tr><td>1 mM</td><td>3.6560 mL</td><td>18.2802 mL</td><td>36.5604 mL</td></tr><tr><td>5 mM</td><td>0.7312 mL</td><td>3.6560 mL</td><td>7.3121 mL</td></tr><tr><td>10 mM</td><td>0.3656 mL</td><td>1.8280 mL</td><td>3.6560 mL</td></tr></table> | Preparing<br>Stock Solutions | <div>Solvent<br/>Concentration</div> <div>Mass</div> | 1 mg       | 5 mg       | 10 mg | 1 mM | 3.6560 mL | 18.2802 mL | 36.5604 mL | 5 mM | 0.7312 mL | 3.6560 mL | 7.3121 mL | 10 mM | 0.3656 mL | 1.8280 mL | 3.6560 mL |
| Preparing<br>Stock Solutions                                                  | <div>Solvent<br/>Concentration</div> <div>Mass</div>                                                                                                                                                                                                                                                                                                                                                                  |                              | 1 mg                                                 | 5 mg       | 10 mg      |       |      |           |            |            |      |           |           |           |       |           |           |           |
|                                                                               | 1 mM                                                                                                                                                                                                                                                                                                                                                                                                                  |                              | 3.6560 mL                                            | 18.2802 mL | 36.5604 mL |       |      |           |            |            |      |           |           |           |       |           |           |           |
|                                                                               | 5 mM                                                                                                                                                                                                                                                                                                                                                                                                                  |                              | 0.7312 mL                                            | 3.6560 mL  | 7.3121 mL  |       |      |           |            |            |      |           |           |           |       |           |           |           |
|                                                                               | 10 mM                                                                                                                                                                                                                                                                                                                                                                                                                 | 0.3656 mL                    | 1.8280 mL                                            | 3.6560 mL  |            |       |      |           |            |            |      |           |           |           |       |           |           |           |
| Please refer to the solubility information to select the appropriate solvent. |                                                                                                                                                                                                                                                                                                                                                                                                                       |                              |                                                      |            |            |       |      |           |            |            |      |           |           |           |       |           |           |           |
| In Vivo                                                                       | 1. Add each solvent one by one: PBS<br>Solubility: 100 mg/mL (365.60 mM); Clear solution; Need ultrasonic                                                                                                                                                                                                                                                                                                             |                              |                                                      |            |            |       |      |           |            |            |      |           |           |           |       |           |           |           |
|                                                                               | 2. Add each solvent one by one: 5% DMSO >> 40% PEG300 >> 5% Tween-80 >> 50% saline<br>Solubility: ≥ 2.5 mg/mL (9.14 mM); Clear solution                                                                                                                                                                                                                                                                               |                              |                                                      |            |            |       |      |           |            |            |      |           |           |           |       |           |           |           |
|                                                                               | 3. Add each solvent one by one: 5% DMSO >> 95% (20% SBE-β-CD in saline)<br>Solubility: ≥ 2.5 mg/mL (9.14 mM); Clear solution                                                                                                                                                                                                                                                                                          |                              |                                                      |            |            |       |      |           |            |            |      |           |           |           |       |           |           |           |
|                                                                               |                                                                                                                                                                                                                                                                                                                                                                                                                       |                              |                                                      |            |            |       |      |           |            |            |      |           |           |           |       |           |           |           |

### BIOLOGICAL ACTIVITY

|                           |                                                                                                                                                                                                                                                                                                |
|---------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Description               | Epetraborole (GSK2251052) hydrochloride is a novel leucyl-tRNA synthetase (LeuRS) inhibitor (IC <sub>50</sub> =0.31 μM), thereby inhibiting protein synthesis. Epetraborole hydrochloride can be used in multidrug-resistant gram-negative pathogens infection research <sup>[1][2][3]</sup> . |
| IC <sub>50</sub> & Target | IC <sub>50</sub> : 0.31 μM (LeuRS) <sup>[3]</sup>                                                                                                                                                                                                                                              |
| In Vitro                  | Epetraborole (0-32 μg/mL) shows anti-bacterial activity against key gram-negative aerobic and anaerobic pathogens and                                                                                                                                                                          |

gram-positive anaerobes<sup>[1]</sup>.

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

Cell Viability Assay<sup>[1]</sup>

|                  |                                                                                                               |
|------------------|---------------------------------------------------------------------------------------------------------------|
| Cell Line:       | Anaerobes isolates                                                                                            |
| Concentration:   | 0-32 µg/mL                                                                                                    |
| Incubation Time: |                                                                                                               |
| Result:          | Showed MIC <sub>50</sub> /MIC <sub>90</sub> for all anaerobes isolates tested of 2 and 4 µg/mL, respectively. |

## CUSTOMER VALIDATION

- Antimicrob Agents Chemother. 2023 Jan 23;e0145922.
- Antimicrob Agents Chemother. 2021 Jul 19;AAC0115621.

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

## REFERENCES

[1]. Goldstein EJ, et al. Comparative in vitro activities of GSK2251052, a novel boron-containing leucyl-tRNA synthetase inhibitor, against 916 anaerobic organisms. Antimicrob Agents Chemother. 2013 May;57(5):2401-4.

[2]. O'Dwyer K, et al. Bacterial resistance to leucyl-tRNA synthetase inhibitor GSK2251052 develops during treatment of complicated urinary tract infections. Antimicrob Agents Chemother. 2015 Jan;59(1):289-98.

[3]. Sutcliffe JA. Antibiotics in development targeting protein synthesis. Ann N Y Acad Sci. 2011 Dec;1241:122-52.

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

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