## **Product** Data Sheet

## BPH-1358 free base

 Cat. No.:
 HY-118946A

 CAS No.:
 801985-13-7

 Molecular Formula:
 C<sub>32</sub>H<sub>28</sub>N<sub>6</sub>O<sub>2</sub>

Molecular Weight: 528.6

Target: Bacterial

Pathway: Anti-infection

Storage: Please store the product under the recommended conditions in the Certificate of

Analysis.

## **BIOLOGICAL ACTIVITY**

Description	BPH-1358 free base (NSC50460 free base) is a potent human farnesyl diphosphate synthase (FPPS) and undecaprenyl diphosphate synthase (UPPS) inhibitor with IC $_{50}$ s of 1.8 $\mu$ M and 110 nM, respectively, and is active against <i>S. aureus</i> in vitro (MIC ~250 ng/mL) $^{[1][2]}$ .
IC <sub>50</sub> & Target	IC50: 1.8 $\mu$ M (human bisphosphonate farnesyl diphosphate synthase)[1]; 100 nM (undecaprenyl diphosphate synthase)[2]
In Vitro	BPH-1358 is the most potent inhibitor of both E. coli UPPS (EcUPPS) as well as S. aureus UPPS (SaUPPS) with an IC $_{50}$ of 110 nM. BPH-1358 against E. coli and S. aureus with EC $_{50}$ of 300 nM and 290 nM, respectively <sup>[1]</sup> . MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	BPH-1358 is active against S. aureus in vivo (20/20 mice survived in an i.p. infection model with a MRSA strain) <sup>[1]</sup> . MCE has not independently confirmed the accuracy of these methods. They are for reference only.

## **REFERENCES**

[1]. Liu YL, et al. Farnesyl diphosphate synthase inhibitors with unique ligand-binding geometries. ACS Med Chem Lett. 2015 Jan 29;6(3):349-54.

[2]. Zhu W, et al. Antibacterial drug leads: DNA and enzyme multitargeting. J Med Chem. 2015 Feb 12;58(3):1215-27.

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

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