## **Product** Data Sheet

# Ethylhydrocupreine hydrochloride

Cat. No.: HY-136429A CAS No.: 3413-58-9 Molecular Formula:  $C_{21}H_{29}CIN_2O_2$  Molecular Weight: 376.92

Target: Bacterial; Parasite

Pathway: Anti-infection

Storage: 4°C, sealed storage, away from moisture and light

\* In solvent: -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture

and light)

**HCI** 

### **SOLVENT & SOLUBILITY**

In Vitro

DMSO: 125 mg/mL (331.64 mM; Need ultrasonic) H<sub>2</sub>O: 50 mg/mL (132.65 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	2.6531 mL	13.2654 mL	26.5308 mL
	5 mM	0.5306 mL	2.6531 mL	5.3062 mL
	10 mM	0.2653 mL	1.3265 mL	2.6531 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

- 1. Add each solvent one by one: PBS Solubility: 33.33 mg/mL (88.43 mM); Clear solution; Need ultrasonic
- 2. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 2.08 mg/mL (5.52 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.08 mg/mL (5.52 mM); Clear solution

### **BIOLOGICAL ACTIVITY**

Description

Ethylhydrocupreine hydrochloride (Optochin hydrochloride) is a quinine derivate with antimicrobial activity against *S. pneumoniae*. Ethylhydrocupreine hydrochloride also possesses antimalarial activity against *Plasmodium falciparum*, with an IC<sub>50</sub> of 25.75 nM. Ethylhydrocupreine hydrochloride is a *Gallus gallus* taste 2 receptors (ggTas2r1, ggTas2r2 and ggTas2r7) agonist<sup>[1][2][3][4]</sup>.

IC<sub>50</sub> & Target

S. pneumoniae $^{[1]}$ 

IC50: 25.75 nM (Plasmodium falciparum)<sup>[3]</sup>

	ggTas2r1, ggTas2r2 and ggTas2r7 <sup>[4]</sup>
In Vitro	The mutation rate to Ethylhydrocupreine (Optochin) resistance is estimated using fluctuation analysis in three capsulated S. pneumoniae strains (S. pneumoniae D39 NCTC 7466, S. pneumoniae R6 ATCC BAA-255 and S. pneumoniae ATCC 49619). The exposure to subinhibitory concentrations of penicillin increased the mutation rate (expressed as mutation per cell division) to Ethylhydrocupreine (Optochin) resistance between 2.1- and 3.1-fold for all three strains studied <sup>[2]</sup> . MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	The injection of 1 cc. of a 24 hour dextrose blood broth culture of virulent Type I pneumococci into the right pleural cavity of guinea pigs produces acute suppurative pleuritis on both sides associated with suppurative pericarditis. The injection of 1 cc. of 1:500 solutions of Ethylhydrocupreine hydrochloride into each pleural cavity of guinea pigs at varying intervals up to 24 hours after pleural infection has usually shown a marked curative influence. Similar results are observed with dogs <sup>[1]</sup> . MCE has not independently confirmed the accuracy of these methods. They are for reference only.

#### **REFERENCES**

- [1]. J A Kolmer, et al. CHEMOTHERAPEUTIC STUDIES WITH ETHYLHYDROCUPREINE HYDROCHLORIDE IN EXPERIMENTAL PNEUMOCOCCUS PLEURITIS. J Exp Med. 1921 May 31;33(6):693-711.
- [2]. Paulo R Cortes, et al. Subinhibitory Concentrations of Penicillin Increase the Mutation Rate to Optochin Resistance in Streptococcus Pneumoniae. J Antimicrob Chemother. 2008 Nov;62(5):973-7.
- [3]. Nassira Mahmoudi, et al. Identification of New Antimalarial Drugs by Linear Discriminant Analysis and Topological Virtual Screening. J Antimicrob Chemother. 2006 Mar;57(3):489-97.
- [4]. Antonella Di Pizio, et al. Molecular Features Underlying Selectivity in Chicken Bitter Taste Receptors. Front Mol Biosci. 2018 Jan 31;5:6.

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

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