Data Sheet (Cat.No.T40417)

TargetMol

Ethylhydrocupreine hydrochloride

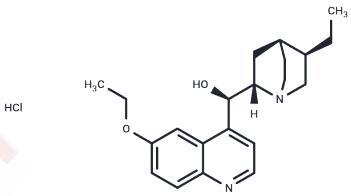
Chemical Properties

CAS No. : 3413-58-9

Formula: C21H29ClN2O2

Molecular Weight: 376.92

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.



Biological Description

Description	Ethylhydrocupreine hydrochloride (Optochin hydrochloride) is a derivative of quinine with antimicrobial activity against Streptococcus pneumoniae and antimalarial activity with an IC50 of 25.75 nM against Plasmodium falciparum. It is also an agonist of Gallus gallus2 receptors (ggTas2r1, ggTas2r2, and ggTas2r7).
Targets(IC50)	Antibacterial,Parasite
In vitro	The mutation rate towards Ethylhydrocupreine (Optochin) resistance in three capsulated S. pneumoniae strains (S. pneumoniae D39 NCTC 7466, S. pneumoniae R6 ATCC BAA-255, and S. pneumoniae ATCC 49619) was determined through fluctuation analysis. It was found that for these strains, subinhibitory concentrations of penicillin noticeably increased the mutation rate (measured as mutations per cell division) to Ethylhydrocupreine (Optochin) resistance, with an enhancement ranging from 2.1- to 3.1-fold [2].
In vivo	The highest tolerated dose of ethylhydrocupreine hydrochloride for guinea pigs by intrapleural injection is about 0.2 to 0.3 cc. of a 1:100 solution per 100 gm. of weight, corresponding to 2 to 3 cc. of solution or 0.02 to 0.03 gm. of the drug per kilo of weight. 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 [1] .

Solubility Information

Solubility	H2O: 50 mg/mL (132.65 mM),Sonication is recommended. DMSO: 125 mg/mL (331.64 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 4 mg/mL (10.61 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
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
50 mM	0.0531 mL	0.2653 mL	0.5306 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

J A Kolmer, et al. CHEMOTHERAPEUTIC STUDIES WITH ETHYLHYDROCUPREINE HYDROCHLORIDE IN EXPERIMENTAL PNEUMOCOCCUS PLEURITIS. J Exp Med. 1921 May 31;33(6):693-711.

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.

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.

Antonella Di Pizio, et al. Molecular Features Underlying Selectivity in Chicken Bitter Taste Receptors. Front Mol Biosci. 2018 Jan 31;5:6.