Benzyldodecyldimethylammonium chloride dihydrate

Cat. No.: HY-128384

CAS No.: 147228-80-6

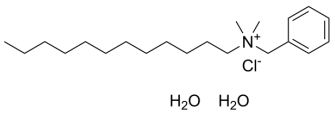
Molecular Formula: $C_{21}H_{42}ClNO_2$

Molecular Weight: 376.02

Target: Bacterial

Pathway: Anti-infection

Storage: 4°C, stored under nitrogen, away from moisture
* In solvent : -80°C, 6 months; -20°C, 1 month (stored under nitrogen, away from moisture)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (265.94 mM; Need ultrasonic)
H_2O : ≥ 100 mg/mL (265.94 mM)
* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.6594 mL	13.2972 mL	26.5943 mL
5 mM	0.5319 mL	2.6594 mL	5.3189 mL
10 mM	0.2659 mL	1.3297 mL	2.6594 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (6.65 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (6.65 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (6.65 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Benzyldodecyldimethylammonium chloride dihydrate is a quaternary ammonium compound (QAC) and can be used as a biocide to target antibiotic-resistant bacteria, such as methicillin-resistant Staphylococcus aureus (MRSA), multidrug-resistant (MDR) P. aeruginosa et. al. Benzyldodecyldimethylammonium chloride dihydrate, an antimicrobial agent, bacteriostatic or bactericidal properties depending on the concentration.

IC_{50} & Target

MIC: 20 mg/L (P. fluorescens)[1]

In Vitro

Benzyldodecyldimethylammonium chloride dihydrate (1-10 μM; 2 hours) results in a dose-dependent changes in the percent population of dead rat thymocyte cells[1].

Benzyldodecyldimethylammonium chloride dihydrate (0-40 mg/L; 0-24 hours) inhibits P. fluorescens with a MIC of 20 mg/L. At 5 mg/L, cells have the same growth behaviour as the control. At concentrations of 10 and 15 mg/L the growth profile is different from the control, and the cells start to grow only after 8 h of adaptation. At concentrations of ≥20 mg/L, BDMDAC inhibits cell growth[2].

Benzyldodecyldimethylammonium chloride dihydrate interacts strongly with cell surfaces in a concentration-dependent manner, and binds by ionic and hydrophobic interactions to microbial membrane surfaces, as manifested by phenomena such as membrane disruption and loss of membrane integrity with consequent leakage of essential intracellular constituents, which promote significant and irreversible changes in the cell structure[2].

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

Cell Viability Assay[1]

Cell Line:	Rat thymocyte cells
Concentration:	0, 5, 10, 15, 20 and 40 mg/L
Incubation Time:	2 hours
Result:	Resulted in cell death.

Cell Proliferation Assay[1]

Cell Line:	Bacterial P. fluorescen
Concentration:	0, 5, 10, 15, 20 and 40 mg/L
Incubation Time:	2 hours
Result:	Inhibited bacterial growth in a time and dose dependent manner.

REFERENCES

[1]. Sadegh Ghanbar, et al. New Generation of N-Chloramine/QAC Composite Biocides: Efficient Antimicrobial Agents To Target Antibiotic-Resistant Bacteria in the Presence of Organic Load. ACS Omega. 2018 Aug 22;3(8):9699-9709.

[2]. Tsuyoshi Mitani, et al. Zinc-related actions of sublethal levels of benzalkonium chloride: Potentiation of benzalkonium cytotoxicity by zinc. Chem Biol Interact. 2017 Apr 25;268:31-36.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA