Benzethonium chloride

Cat. No.: HY-B0942

CAS No.: 121-54-0

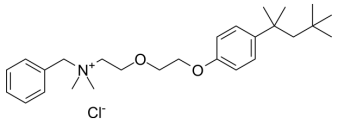
Molecular Formula: $C_{27}H_{42}ClNO_2$

Molecular Weight: 448.08

Target: nAChR; Bacterial; Apoptosis; Caspase

Pathway: Membrane Transporter/Ion Channel; Neuronal Signaling; Anti-infection; Apoptosis

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)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 33.33 mg/mL (74.38 mM; Need ultrasonic)
H_2O : 20 mg/mL (44.63 mM; Need ultrasonic)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	2.2317 mL	11.1587 mL	22.3174 mL
	5 mM	0.4463 mL	2.2317 mL	4.4635 mL
	10 mM	0.2232 mL	1.1159 mL	2.2317 mL

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

In Vivo

1. Add each solvent one by one: PBS
   Solubility: 120 mg/mL (267.81 mM); Clear solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (5.58 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (5.58 mM); Clear solution
4. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (5.58 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Benzethonium chloride inhibits nicotinic acetylcholine receptors in human recombinant α7 and α4β2 neurons in Xenopus laevis oocytes, which has antibacterial, anticancer, antisepsis and disinfection activity. Benzethonium chloride induced Apoptosis and activated caspases in cancer cell lines. Benzethonium chloride ablates the tumor-forming ability of FaDu cells, delays the growth of xenograft tumors in vivo[1][2][3].

In Vitro

Benzethonium chloride (0.1 g/L, 10 s) results in only a 50% reduction in bacterial number against S. mutans MT8148 and Streptococcus sobrinus[1].
Benzethonium chloride (0.1-100 μM, 48 h) reduces cell viability against FaDu and C666-1 (both human cancer) cell lines with EC_{50} values of 3.8 and 5.3 μM, respectively[2].
Benzethonium chloride (9 μM, 24-48 h) induces apoptosis and caspase activation in FaDu cells[2].
Benzethonium chloride (0.1 and 5 mg/L, 24-72 h) shows great acute toxicity to C. elegans, induces an inhibition on hatching and increases mortality in zebrafish embryos[3].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Apoptosis Analysis[2]

Cell Line:	FaDu cells
Concentration:	9 μM
Incubation Time:	24-48 h
Result:	Revealed nuclear condensation and blebbing and Caspase-2, caspase-8, and caspase-9 activations, indicative of apoptosis, after 48 hours of treatment.

In Vivo

Benzethonium chloride (5 mg/kg, i.p., daily for 5 days) results in elimination of tumor formation and growth delay in established xenograft tumors[2].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Established xenograft tumors of mice[2]
Dosage:	5 mg/kg
Administration:	i.p., daily for 5 days
Result:	Effectively eliminates the tumorforming potential of FaDu cells and survived for 3.5 days more than PBS-treated mice, which was a statistically significant delay.

REFERENCES

[1]. Maillard JY. Impact of benzalkonium chloride, benzethonium chloride and chloroxylenol on bacterial antimicrobial resistance. J Appl Microbiol. 2022 Dec;133(6):3322-3346.

[2]. Yip KW, et al. Benzethonium chloride: a novel anticancer agent identified by using a cell-based small-molecule screen. Clin Cancer Res. 2006 Sep 15;12(18):5557-69.

[3]. Sreevidya VS, et al. Benzalkonium chloride, benzethonium chloride, and chloroxylenol - Three replacement antimicrobials are more toxic than triclosan and triclocarban in two model organisms. Environ Pollut. 2018 Apr;235:814-824.

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