Clofoctol

Cat. No.: HY-B1150

CAS No.: 37693-01-9

Molecular Formula: $C_{21}H_{26}Cl_2O$

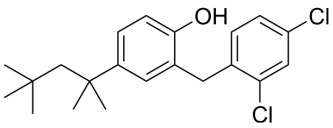
Molecular Weight: 365.34

Target: Bacterial; Antibiotic; SARS-CoV

Pathway: Anti-infection

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (273.72 mM; Need ultrasonic)

H_2O : < 0.1 mg/mL (insoluble)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.7372 mL	13.6859 mL	27.3718 mL
5 mM	0.5474 mL	2.7372 mL	5.4744 mL
10 mM	0.2737 mL	1.3686 mL	2.7372 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 (6.84 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.5 mg/mL (6.84 mM); Suspended solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (6.84 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Clofoctol is a bacteriostatic antibiotic. Clofoctol is used in the treatment of respiratory tract and ear, nose and throat infections caused by Gram-positive bacteria. Clofoctol is only functional against Gram-positive bacteria and can penetrate into human lung tissue. Clofoctol is also an inhibitor of prostate cancer. Clofoctol has antiviral potency[1][2][3].

In Vitro

Clofoctol (0-100 μM; 72 h) inhibits prostate cancer cell growth[2].

Clofoctol (0-20 μM; 24 h) arrests cell cycle at G_1 phase[2].

Clofoctol (0-30 μM; 0-24 h) induces ER stress and activates UPR pathways[2].
Clofoctol (0-40 μM; 24 h) inhibits translation[2].
Clofoctol (0-100 μM; 24 h) shows antiviral effect against SARS-CoV-2 with IC_{50}s of 9.3 μM and 11.59 μM in Vero-81 and Vero-81-TMPRSS2 cells, respectively[3].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Viability Assay[2]

Cell Line:	Prostate cancer cell lines: LNCaP, DU145, PC3, LAPC4, CWR22Rv1 and C42B
Concentration:	0-100 μM
Incubation Time:	72 h
Result:	Inhibited cell growth with IC_{50} values ranging from 10 to 15 μM.

Cell Viability Assay[2]

Cell Line:	PC3
Concentration:	0, 10 and 20 μM
Incubation Time:	24 h
Result:	Induced a G_1 arrest.

RT-PCR[2]

Cell Line:	PC3
Concentration:	0, 5, 10, 15, 20 and 30 μM
Incubation Time:	24 h
Result:	Increased the splicing of XBP-1 mRNA in PC3 cells in a dose-dependent manner. Dose-dependently decreased PstI digestion products from XBP-1 mRNA.

Western Blot Analysis[2]

Cell Line:	PC3
Concentration:	0, 5, 10, 15, 20, 25 and 30 μM
Incubation Time:	0, 0.5, 1, 3, 6 and 9 h or 24 h (cell cycle)
Result:	Dose- and time-dependently increased the level of phosphorylated eIF2α, up-regulated CHOP expression, and increased the expression of BiP. Led to a dose-dependent decrease in the levels of cyclin A and cyclin D1.

In Vivo

Clofoctol (175 mg/kg; i.p.; daily for 37 days) is capable of blocking tumour growth without apparent toxicity in a mouse model of human prostate cancer xenograft[2].
Clofoctol (62.5 mg/kg; i.p.; twice) inhibits SARS-CoV-2 replication and lowers inflammation in lungs in mice with SARS-CoV-2 infection[3].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Male athymic nude mice (BALB/c, nu/nu-NCr) aged 4–6 weeks, human prostate cancer xenograft model[2]

Dosage:	175 mg/kg
Administration:	Intraperitoneal injection, daily for 37 days
Result:	Significantly inhibited PC3 tumour growth, tumour weight was also reduced by 60%.

Animal Model:	K18-hACE2 transgenic C57BL/6J mice with SARS-CoV-2 infection[3]
Dosage:	62.5 mg/kg
Administration:	Intraperitoneal injection, 1h and 8h post-infection
Result:	Induced body weight loss, reduced the viral load in the lungs. The expression of transcripts encoding IL-6, TNFα, IL12p40, IFNβ, IFNγ and the interferon-stimulated genes (ISG) Mx1, Ifi44 and ISG15 was markedly reduced.

Animal Model:	8–10 week-old female C57BL/6J mice[3]
Dosage:	62.5mg/kg
Administration:	Intraperitoneal injection, once (Pharmacokinetics)
Result:	Reached concentrations up to 61 μM in the lungs and remained above this level for almost 4h as early as 30 min after injection.

REFERENCES

[1]. Belouzard S, et al. Clofoctol inhibits SARS-CoV-2 replication and reduces lung pathology in mice. PLoS Pathog. 2022 May 19;18(5):e1010498.

[2]. Ghilardi PL, et al. Treatment of ear, nose and throat infections with clofoctol. Drugs Exp Clin Res. 1985;11(11):815-8.

[3]. Wang M, et al. Identification of an old antibiotic clofoctol as a novel activator of unfolded protein response pathways and an inhibitor of prostate cancer. Br J Pharmacol. 2014 Oct;171(19):4478-89.

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