Data Sheet (Cat.No.T208293)

TargetMol

Antibacterial agent 166

Chemical Properties

CAS No. :

Formula: C11H8ClN3O4

Molecular Weight:

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	Antibacterialagent 166 is a derivative of Nitishinone, functioning as a selective and orally active inhibitor of Fusobacterium nucleatum with an MIC50 of 1 μg/mL. It effectively reduces the migration capability of MC-38 cells induced by Fusobacterium nucleatum. Antibacterialagent 166 is a promising lead compound for studying colorectal cancer (CRC) due to its anti-F. nucleatum properties.
Targets(IC50)	Antibacterial
In vitro	Antibacterial agent 166 (Compound 19q) at concentrations of 1-4 μg/mL inhibits the growth and biofilm formation of Fusobacterium nucleatum in a dose-dependent manner over 0-72 hours. It suppresses the bacterium's growth by downregulating NTR expression when used at 1-4 μg/mL for 4-48 hours and decreases the expression of the tnaA gene in a dose-dependent manner during the late logarithmic phase at 1-4 μg/mL for 48 hours. Additionally, in the presence of Fusobacterium nucleatum, Antibacterial agent 166 at 2-4 μg/mL for 48 hours strongly inhibits the migration of MC-38 cells, demonstrating effective inhibitory activity with an IC50 of 11 μM. For two human normal cell lines, it exhibits moderate to weak antiproliferative activity with an IC50 of 16 μM, indicating lower cytotoxicity.
In vivo	Antibacterial agent 166 (Compound 19q) at a dose of 1500 mg/kg (single administration) demonstrates minimal toxic effects on organs. When administered orally at 20 mg/kg (single-dose), it effectively localizes in the intestines to inhibit Fusobacterium nucleatum, with low systemic toxicity. For intravenous administration at 1 mg/kg, the agent's half-life is approximately 0.068 hours, with a peak concentration (C max) of 85 ng/mL and a plasma clearance rate (CL) of 36054 mL/h/mg.

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