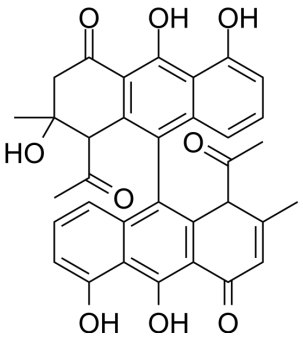
Setomimycin

Cat. No.:	HY-124439
CAS No.:	69431-87-4
Molecular Formula:	$C_{34}H_{28}O_9$
Molecular Weight:	580.58
Target:	Antibiotic; Bacterial; SARS-CoV
Pathway:	Anti-infection
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	Setomimycin is a potent antibiotic. Setomimycin inhibits the SARS-CoV-2 Mpro enzyme with an IC_{50} value of 12.02 μM. Setomimycin shows anti-inflammatory and antioxidant properties. Setomimycin shows antiproliferative and antitumor activity[1][2].
IC_{50} & Target	IC_{50}: 12.02 μM (SARS-CoV-2 Mpro)[1]
In Vitro	Setomimycin (0.01-1 μM) inhibits the release of cytokines IL-1β, IL-6 and TNF-α and nitric oxide release from LPS stimulated RAW 264.7 cells in a dose-dependent manner[1]. Setomimycin (compound 1) shows antimicrobial activity with MICs of 8, 4, 16, 4 μg/mL for Staphylococcus aureus, Bacillus cereus, Bacillus subtilis, Micrococcus luteus, respectively[2]. Setomimycin (0-100 μM; 5 days) shows antiproliferative activity and inhibits colony formation[2]. Setomimycin (4, 5.5, 7 μM) decreases the protein expression of p-MEK, p-ERK, Bcl-2, increases the expression of Par-4[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Proliferation Assay[2]

Cell Line:	A549; HOP-92; Panc-1; MiaPaca-2 cells
Concentration:	0-100 μM
Incubation Time:	44 h
Result:	Showed antiproliferative activity with IC_{50}s of 11.45, >100, 48, 4.57 μM for A549; HOP-92; Panc-1; MiaPaca-2 cells, respectively.

Western Blot Analysis[2]

Cell Line:	MCF-7, HCT-116 cells
Concentration:	4, 5.5, 7 μM
Incubation Time:	
Result:	Decreased the protein expression of p-MEK, p-ERK, Bcl-2, increased the expression of Par-4 in a dose-dependent manner.

In Vivo

Setomimycin (20 mg/kg; i.p.; alternate days for two weeks) shows antitumor activity in mice[2].

Pharmacokinetic Parameters of Setomimycin in female BALB/c mice[2].

Pharmacokinetic parameters	Value
C_{max} (ng/ml)	694 ± 62
T_{max} (h)	0.3 ± 0.1
$T_{1/2}$ (h)	2.3 ± 0.5
AUC_{0-t} (ng.h/mL)	2613 ± 111
$AUC_{0-\alpha}$ (ng.h/mL)	2734 ± 108
V_d (L/Kg)	24 ± 4
Cl (L/h/Kg)	7.4 ± 0.3

Female BALB/c mice, 20 mg/kg ip (1 % DMSO +30 % PEG-200 + 2 % Tween 80 + q.s. water (v/v))[2]

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

Animal Model:	6 weeks, 25-30 g, female BALB/c mice (4T1 cells)[2]
Dosage:	20 mg/kg
Administration:	I.p.; every other day for two weeks
Result:	Decreased primary tumor weight (76%) and volume (90.5%).

REFERENCES

[1]. Manhas RS, et al. Setomimycin as a potential molecule for COVID‐19 target: in silico approach and in vitro validation. Mol Divers. 2023 Apr;27(2):619-633.

[2]. Manhas RS, et al. Isolation and anticancer activity evaluation of rare Bisaryl anthraquinone antibiotics from novel Streptomyces sp. strain of NW Himalayan region. Chem Biol Interact. 2022 Sep 25;365:110093.

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