Duocarmycin DM free base

Cat. No.: HY-128915

CAS No.: 1116745-06-2

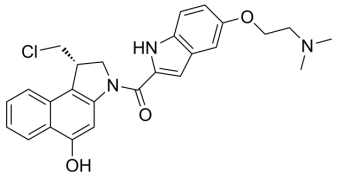
Molecular Formula: $C_{26}H_{26}ClN_3O_3$

Molecular Weight: 463.96

Target: DNA Alkylator/Crosslinker; ADC Cytotoxin

Pathway: Cell Cycle/DNA Damage; Antibody-drug Conjugate/ADC Related

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



SOLVENT & SOLUBILITY

In Vitro

DMSO : 50 mg/mL (107.77 mM; Need ultrasonic)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	2.1554 mL	10.7768 mL	21.5536 mL
	5 mM	0.4311 mL	2.1554 mL	4.3107 mL
	10 mM	0.2155 mL	1.0777 mL	2.1554 mL

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

BIOLOGICAL ACTIVITY

Description

Duocarmycin DM free base, a DNA minor-groove alkylator, is an antibody agent conjugates (ADCs) toxin. Duocarmycin DM free base is based on its characteristic curved indole structure and a spirocyclopropylcyclohexadienone electrophile to act anticancer activity[1][2].

IC_{50} & Target

Daunorubicins/Doxorubicins

In Vitro

The Duocarmycins and CC-1065 are members of a class of DNA minor groove, AT-sequence selective, and adenine-N3 alkylating agents, isolated from Streptomyces sp. that exhibit extremely potent cytotoxicity against the growth of cancer cells grown in culture[2].

Duocarmycin shows cytotoxicity to several human cancer cells, with IC_{50} of 22, 13.8, 3.87, 15.4, and 7.31 pM for HT-29, CL1-5, Caski, EJ, and LS174T, respectively[3].

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

REFERENCES

[1]. Patil PC, et al. A Short Review on the Synthetic Strategies of Duocarmycin Analogs that are Powerful DNA Alkylating Agents. Anticancer Agents Med Chem. 2015;15(5):616-630.

[2]. Koch MF, et al. Structural, Biochemical, and Computational Studies Reveal the Mechanism of Selective Aldehyde Dehydrogenase 1A1 Inhibition by Cytotoxic Duocarmycin Analogues. Angew Chem Int Ed Engl. 2015 Nov 9;54(46):13550-4.

[3]. Chen KC, et al. Selective cancer therapy by extracellular activation of a highly potent glycosidic duocarmycin analogue. Mol Pharm. 2013;10(5):1773-1782.

[4]. Chen KC, Schmuck K, Tietze LF, Roffler SR. Selective cancer therapy by extracellular activation of a highly potent glycosidic duocarmycin analogue. Mol Pharm. 2013;10(5):1773-1782.

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