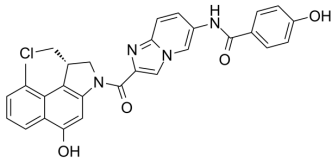
Seco-DUBA

Cat. No.:	HY-132180A
CAS No.:	1227961-59-2
Molecular Formula:	$C_{29}H_{23}ClN_4O_4$
Molecular Weight:	526.97
Target:	ADC Cytotoxin
Pathway:	Antibody-drug Conjugate/ADC Related
Storage:	-20°C, stored under nitrogen * In solvent : -80°C, 6 months; -20°C, 1 month (stored under nitrogen)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (189.76 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.8976 mL	9.4882 mL	18.9764 mL
	5 mM	0.3795 mL	1.8976 mL	3.7953 mL
	10 mM	0.1898 mL	0.9488 mL	1.8976 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: 1 mg/mL (1.90 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 1 mg/mL (1.90 mM); Suspended solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

Seco-DUBA is a duocarmycin (DUBA) prodrug containing two hydroxyl groups, which can each be used for coupling to an antibody via a linker. Seco-DUBA can be used in the synthesis of antibody-drug conjugates (ADCs)[1].

In Vitro

Seco-DUBA (SK-BR-3 cells; 0.0001 pM~0.01 nM; 144 hours) dose-dependent reduces cell viability and shows equally potent and efficacious as DUBA[1].

Seco-DUBA causes SK-BR-3 (IC_{50}=0.09), SK-OV-3 (IC_{50}=0.43), and SW620 (IC_{50}=0.09) cells to exhibit highly sensitive[1].

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

Cell Cytotoxicity Assay[1]

Cell Line:	SK-BR-3 cells

Concentration:	0.0001 pM~0.01 nM
Incubation Time:	144 hours
Result:	Dose-dependent reduced cell viability.

In Vivo

Seco-DUBA (89 μg/kg; i.v.) is likely converted to DUBA almost instantaneously[1].

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

Animal Model:	Wistar rats[1]
Dosage:	89 μg/kg (Pharmacokinetic Analysis)
Administration:	I.v.
Result:	Likely converted to DUBA almost instantaneously.

REFERENCES

[1]. Elgersma RC, et al. Design, Synthesis, and Evaluation of Linker-Duocarmycin Payloads: Toward Selection of HER2-Targeting Antibody-Drug Conjugate SYD985. Mol Pharm. 2015;12(6):1813-1835.

[2]. Platform Technologies in Drug Discovery and Validation

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