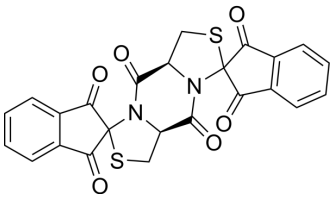
ZINC03129319

Cat. No.:	HY-112254
CAS No.:	1777807-64-3
Molecular Formula:	$C_{24}H_{14}N_2O_6S_2$
Molecular Weight:	490.51
Target:	Virus Protease; Flavivirus; Dengue virus
Pathway:	Anti-infection
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 41.67 mg/mL (84.95 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.0387 mL	10.1935 mL	20.3869 mL
	5 mM	0.4077 mL	2.0387 mL	4.0774 mL
	10 mM	0.2039 mL	1.0193 mL	2.0387 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: 2.08 mg/mL (4.24 mM); Clear solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.08 mg/mL (4.24 mM); Clear solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (4.24 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

ZINC03129319 is a dengue virus (DENV) NS2B-NS3 protease inhibitor extracted from patent US20150141521A1, has inhibition constants (K_{i1}) of 92 μM and K_{i3} of 20 μM.

IC_{50} & Target

Ki1: 92±15 μM (DENV NS2B-NS3 protease)[1]
Ki3: 20±4 μM (DENV NS2B-NS3 protease)[1]

In Vitro

ZINC03129319 inhibits DENV NS2B-NS3 protease with K_{i1} of 92±15 μM and K_{i3} of 20±4 μM[1].

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

REFERENCES

[1]. Watowich, Stanley J, et al. SMALL-MOLECULE INHIBITORS OF DENGUE VIRUS PROTEASES. US20150141521A1.

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