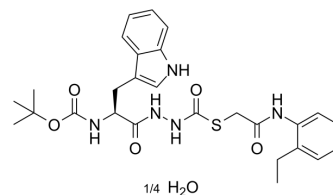


SID 26681509 quarterhydrate

Cat. No.:	HY-103353A
Molecular Formula:	C ₂₇ H ₃₃ N ₅ O ₅ S ₁ /4H ₂ O
Molecular Weight:	544.16
Target:	Cathepsin; Parasite
Pathway:	Metabolic Enzyme/Protease; Anti-infection
Storage:	Powder -20°C 3 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro	DMSO : 50 mg/mL (91.88 mM; Need ultrasonic)					
	Ethanol : 5 mg/mL (9.19 mM; Need ultrasonic and warming)					
	Preparing Stock Solutions	Solvent	Mass	1 mg	5 mg	10 mg
		Concentration				
		1 mM		1.8377 mL	9.1885 mL	18.3769 mL
5 mM			0.3675 mL	1.8377 mL	3.6754 mL	
10 mM		0.1838 mL	0.9188 mL	1.8377 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: ≥ 1.67 mg/mL (3.07 mM); Clear solution					

BIOLOGICAL ACTIVITY

Description	SID 26681509 quarterhydrate is a potent, reversible, competitive, and selective inhibitor of human cathepsin L with an IC ₅₀ of 56 nM. SID 26681509 quarterhydrate inhibits in vitro propagation of malaria parasite <i>Plasmodium falciparum</i> and inhibits <i>Leishmania major</i> with IC ₅₀ s of 15.4 μM and 12.5 μM, respectively. SID 26681509 quarterhydrate shows no inhibitory activity against cathepsin G ^[1] .
IC ₅₀ & Target	Plasmodium
In Vitro	After a 4 hr preincubation with cathepsin L, SID 26681509 becomes more potent, demonstrating an IC ₅₀ of 1.0 nM. SID 26681509 is determined to be a slow-binding and slowly reversible competitive inhibitor. Through a transient kinetic analysis for single-step reversibility, inhibition rate constants are kon = 24,000 M ⁻¹ s ⁻¹ and koff = 2.2 × 10 ⁻⁵ s ⁻¹ (K _i = 0.89 nM). Molecular docking studies are undertaken using the experimentally-derived X-ray crystal structure of papain/CLIK-148 ^[1] . SID 26681509 inhibits papain and cathepsins B, K, S, and V with IC ₅₀ values determined after one hour ranging from 618 nM to 8.442 μM. SID 26681509 shows no inhibitory activity against the serine protease cathepsin G ^[1] .

SID 26681509 inhibits cathepsin V activity with an IC₅₀ value of 0.5 μM. SID 26681509 (1-30 μM) blocks high-mobility group box 1 (HMGB1)-induced TNF-α production dose dependently without altering cell viability^[2].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

SID 26681509 treatment significantly improves survival in murine models of sepsis and reduces liver damage following warm liver ischemia/reperfusion (I/R) models^[2].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Signal Transduct Target Ther. 2021 Mar 27;6(1):134.
- Nat Commun. 2022 May 26;13(1):2935.
- Nat Commun. 2020 Mar 27;11(1):1620.

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REFERENCES

[1]. Shah PP, et al. Kinetic characterization and molecular docking of a novel, potent, and selective slow-binding inhibitor of human cathepsin L. Mol Pharmacol. 2008 Jul;74(1):34-41.

[2]. Pribis JP, et al. The HIV Protease Inhibitor Saquinavir Inhibits HMGB1-Driven Inflammation by Targeting the Interaction of Cathepsin V with TLR4/MyD88. Mol Med. 2015 Dec;21(1):749-757.

Caution: Product has not been fully validated for medical applications. For research use only.

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