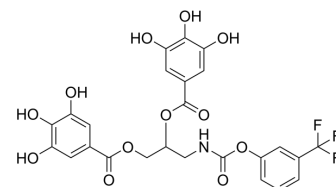


CDE-096

Cat. No.:	HY-120516
CAS No.:	1228357-04-7
Molecular Formula:	C ₂₅ H ₂₀ F ₃ NO ₁₂
Molecular Weight:	583.42
Target:	PAI-1
Pathway:	Metabolic Enzyme/Protease
Storage:	4°C, sealed storage, away from moisture and light * In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture and light)



SOLVENT & SOLUBILITY

In Vitro	DMSO : 100 mg/mL (171.40 mM; Need ultrasonic)				
		Solvent	Mass		
		Concentration	1 mg	5 mg	10 mg
	Preparing Stock Solutions	1 mM	1.7140 mL	8.5702 mL	17.1403 mL
		5 mM	0.3428 mL	1.7140 mL	3.4281 mL
		10 mM	0.1714 mL	0.8570 mL	1.7140 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: ≥ 2.5 mg/mL (4.29 mM); Clear solution				
	2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.5 mg/mL (4.29 mM); Clear solution				
	3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.5 mg/mL (4.29 mM); Clear solution				

BIOLOGICAL ACTIVITY

Description	CDE-096 is a potent inhibitor of PAI-1. CDE-096 prevents PAI-1 from inactivating tPA and uPA with similar potency (IC ₅₀ =30 and 25 nM, respectively) and is active against glycosylated PAI-1, as well as PAI-1 derived from several species (IC ₅₀ =19, 22 and 18 nM for murine, rat, and Porcine PAI-1, respectively) ^[1] .
In Vitro	CDE-096 is active against both free PAI-1 and vitronectin-bound PAI-1. CDE-096 binds to PAI-1 with nanomolar affinity and induces conformational changes that prevent binding to both proteases and vitronectin ^[1] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Li SH, et al. Mechanistic characterization and crystal structure of a small molecule inactivator bound to plasminogen activator inhibitor-1. Proc Natl Acad Sci U S A. 2013;110(51):E4941-E4949.

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

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