Azulene

Cat. No.:	HY-B0055			
CAS No.:	275-51-4			
Molecular Formula:	C ₁₀ H ₈			
Molecular Weight:	128.17			
Target:	HIV			
Pathway:	Anti-infection			
Storage:	Powder	-20°C	3 years	
		4°C	2 years	
	In solvent	-80°C	2 years	
		-20°C	1 year	

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SOLVENT & SOLUBILITY

In Vitro	DMSO : 100 mg/mL (7	80.21 mM; Need ultrasonic)					
	Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg		
		1 mM	7.8021 mL	39.0107 mL	78.0214 mL		
		5 mM	1.5604 mL	7.8021 mL	15.6043 mL		
		10 mM	0.7802 mL	3.9011 mL	7.8021 mL		
	Please refer to the solubility information to select the appropriate solvent.						
In Vivo	1. Add each solvent of Solubility: ≥ 2.5 m	. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 2.5 mg/mL (19.51 mM); Clear solution					
	2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.5 mg/mL (19.51 mM); Clear solution						
	3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.5 mg/mL (19.51 mM); Clear solution						

DIGEOGICALACITY				
Description	Azulene (Cyclopentacycloheptene) is as an isomer of naphthalene with high anti-HIV activity. Azulene, isolated from the distillation of chamomile oil, is a scaffold in medicinal chemistry ^{[1][2][3]} .			
IC ₅₀ & Target	HIV			
In Vitro	Azulene is an interesting scaffold in medicinal chemistry as it resembles several other bicyclic aromatics that are frequently found in drugs. Azulene, a structural isomer of naphthalene, is a bicyclic nonbenzenoid aromatic hydrocarbon having a			

dipole moment due to the electron-rich five-membered ring and electron-deficient sevenmembered ring^[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Teppo O Leino, et al. Azulene-based Compounds for Targeting Orexin Receptors. Eur J Med Chem. 2018 Sep 5;157:88-100.

[2]. Julia Peet, et al. Antiretroviral (HIV-1) Activity of Azulene Derivatives. Bioorg Med Chem. 2016 Apr 15;24(8):1653-7.

[3]. David A. Becker, et al. A new synthesis of substituted azulenes. Journal of the American Chemical Society, 111(1), 389-391.

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

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