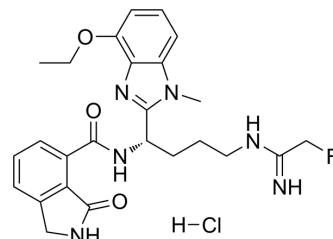


AFM32a hydrochloride

Cat. No.:	HY-136557A
Molecular Formula:	C ₂₅ H ₃₀ ClFN ₆ O ₃
Molecular Weight:	517
Target:	Protein Arginine Deiminase
Pathway:	Epigenetics
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 (193.42 mM; Need ultrasonic)					
	Preparing Stock Solutions	Solvent	Mass	1 mg	5 mg	10 mg
		Concentration				
		1 mM		1.9342 mL	9.6712 mL	19.3424 mL
		5 mM		0.3868 mL	1.9342 mL	3.8685 mL
10 mM		0.1934 mL	0.9671 mL	1.9342 mL		
Please refer to the solubility information to select the appropriate solvent.						
In Vivo	<ol style="list-style-type: none"> Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 2.5 mg/mL (4.84 mM); Clear solution Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.5 mg/mL (4.84 mM); Clear solution Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.5 mg/mL (4.84 mM); Clear solution 					

BIOLOGICAL ACTIVITY

Description	AFM32a (PAD2-IN-1) hydrochloride, a benzimidazole-based derivative, is a potent and selective protein arginine deiminase 2 (PAD2) inhibitor. AFM32a hydrochloride shows superior selectivity for PAD2 over PAD4 (95-fold) and PAD3 (79-fold) ^[1] .
IC₅₀ & Target	Protein Arginine Deiminase 2 (PAD2) ^[1]
In Vitro	In the target engagement assay, the EC ₅₀ of AFM32a (compound 32a) hydrochloride is 8.3 μM in HEK293T/PAD2 cells, the enhanced potency of AFM32a overcomes its relatively poor ability to enter cells ^[1] . AFM32a (compound 32a; 1-25 μM) hydrochloride treatment strongly inhibits histone H3 citrullination with an EC ₅₀ of 2.7 μM in HEK293T/PAD2 cells ^[1] .

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

CUSTOMER VALIDATION

- Front Immunol. 01 December 2021.

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REFERENCES

[1]. Aaron Muth, et al. Development of a Selective Inhibitor of Protein Arginine Deiminase 2. J Med Chem. 2017 Apr 13;60(7):3198-3211.

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

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