

AFM-30a hydrochloride

Cat. No.: HY-125099A Molecular Formula: $\mathsf{C_{24}H_{28}CIFN_6O_3}$

Molecular Weight: 502.97

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)

Product Data Sheet

SOLVENT & SOLUBILITY

In Vitro

DMSO: 50 mg/mL (99.41 mM; ultrasonic and warming and heat to 60°C)

H₂O: 50 mg/mL (99.41 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	1.9882 mL	9.9410 mL	19.8819 mL
	5 mM	0.3976 mL	1.9882 mL	3.9764 mL
	10 mM	0.1988 mL	0.9941 mL	1.9882 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: ≥ 5 mg/mL (9.94 mM); Clear solution
- 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 5 mg/mL (9.94 mM); Clear solution

BIOLOGICAL ACTIVITY

Description	AFM-30a hydrochloride is a potent protein arginine deiminase 2 (PAD2) inhibitor and has excellent PAD2-selectivity. AFM-30a hydrochloride binds to PAD2 with an EC $_{50}$ value of 9.5 μ M. AFM-30a hydrochloride also inhibits H3 citrullination with an EC $_{50}$ value of 0.4 μ M. AFM-30a hydrochloride can be used for the research of certain cancers and a variety of autoimmune diseases including rheumatoid arthritis (RA), multiple sclerosis, lupus, and ulcerative colitis ^[1] .
IC ₅₀ & Target	EC50: 9.5 μ M (PAD2); 0.4 μ M (H3 citrullination) [1]

AFM-30a hydrochloride (compound 30a; 25 μM) has good potency to enter HEK293T/PAD2 cells and covalent modify PAD2 In Vitro with an EC₅₀ of 9.5 μ M^[1].

AFM-30a hydrochloride shows good ability to inhibit H3 citrullination with an EC₅₀ of 0.4 μ M^[1].

	MCE has not independe Cell Viability Assay ^[1]	MCE has not independently confirmed the accuracy of these methods. They are for reference only. $ \text{Cell Viability Assay}^{[1]} $	
	Cell Line:	HEK293T/PAD2 cells	
	Concentration:	Various concentrations	
	Incubation Time:	24 h	
	Result:	Exhibited low cytotoxicity for cells.	
In Minns			
In Vivo	· ·	AFM-30a hydrochloride suppresses NLRP3 signaling and decreases airway remodeling in PAD2 ^{-/-} transgenic mice ^[2] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.	

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.

[2]. R. Surolia, et al. Role of PAD2 Regulated Inflammasome Signaling in Arsenic Induced Airway Inflammation and Remodeling. American Journal of Respiratory and Critical Care Medicine 2020;201:A2976.

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

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