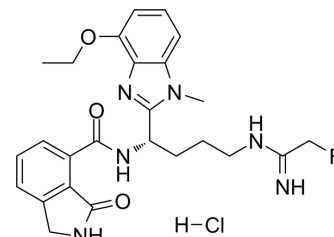


AFM32a hydrochloride

Cat. No.:	HY-136557A
CAS No.:	2988594-85-8
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)																					
	<table border="1"> <thead> <tr> <th rowspan="2">Solvent</th> <th rowspan="2">Mass</th> <th colspan="3">Concentration</th> </tr> <tr> <th>1 mg</th> <th>5 mg</th> <th>10 mg</th> </tr> </thead> <tbody> <tr> <td rowspan="3">Preparing Stock Solutions</td> <td>1 mM</td> <td>1.9342 mL</td> <td>9.6712 mL</td> <td>19.3424 mL</td> </tr> <tr> <td>5 mM</td> <td>0.3868 mL</td> <td>1.9342 mL</td> <td>3.8685 mL</td> </tr> <tr> <td>10 mM</td> <td>0.1934 mL</td> <td>0.9671 mL</td> <td>1.9342 mL</td> </tr> </tbody> </table>	Solvent	Mass	Concentration			1 mg	5 mg	10 mg	Preparing Stock Solutions	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
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	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: PBS Solubility: 12.5 mg/mL (24.18 mM); Clear solution; Need ultrasonic 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 μ M) hydrochloride treatment strongly inhibits histone H3 citrullination with an EC₅₀ of 2.7 μ M 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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