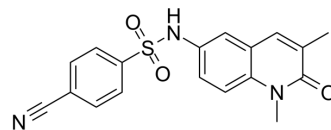


NI-42

Cat. No.:	HY-101121		
CAS No.:	1884640-99-6		
Molecular Formula:	C ₁₈ H ₁₅ N ₃ O ₃ S		
Molecular Weight:	353.4		
Target:	Epigenetic Reader Domain		
Pathway:	Epigenetics		
Storage:	Powder	-20°C	3 years
	In solvent	-80°C	6 months
		-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro	DMSO : 100 mg/mL (282.97 mM; Need ultrasonic)					
	Preparing Stock Solutions	Solvent Concentration	Mass			
			1 mg	5 mg	10 mg	
			1 mM	2.8297 mL	14.1483 mL	28.2965 mL
			5 mM	0.5659 mL	2.8297 mL	5.6593 mL
10 mM	0.2830 mL	1.4148 mL	2.8297 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 (7.07 mM); Clear solution					
	2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: 2.5 mg/mL (7.07 mM); Suspended solution; Need ultrasonic					

BIOLOGICAL ACTIVITY

Description	NI-42 (compound 13-d), a structurally orthogonal chemical probe for the BRPFs, is a biased, potent inhibitor of the BRD of the BRPFs (IC ₅₀ s of BRPF1/2/3=7.9/48/260 nM; K _d s of BRPF1/2/3=40/210/940 nM) with excellent selectivity over nonclass IV BRD proteins ^[1] .			
IC ₅₀ & Target	BRPF1 7.9 nM (IC ₅₀)	BRPF2 48 nM (IC ₅₀)	BRPF3 260 nM (IC ₅₀)	BRPF1 40 nM (K _d)
	BRPF2 210 nM (K _d)	BRPF3 940 nM (K _d)	BRD4 (BD1) 4500 nM (IC ₅₀)	BRD7 82 nM (IC ₅₀)
	BRD9	BRD9		

	310 nM (IC ₅₀)	1130 nM (K _d)
In Vitro	NI-42 shows IC ₅₀ s of 82, 310, and 4500 nM for BRD7, BRD9, and BRD4 (BD1), respectively, and has a K _d of 1130 nM for BRD9 ^[1] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.	

REFERENCES

[1]. Igoe N, et al. Design of a Biased Potent Small Molecule Inhibitor of the Bromodomain and PHD Finger-Containing (BRPF) Proteins Suitable for Cellular and in Vivo Studies. J Med Chem. 2017 Jan 26;60(2):668-680.

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

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