# **Product** Data Sheet

### **DUB-IN-1**

Cat. No.:HY-50736CAS No.:924296-18-4Molecular Formula: $C_{20}H_{11}N_5O$ Molecular Weight:337.33

Target: Deubiquitinase

Pathway: Cell Cycle/DNA Damage

Storage: Powder -20°C 3 years

4°C 2 years

In solvent -80°C 2 years

-20°C 1 year

#### **SOLVENT & SOLUBILITY**

In Vitro

DMSO: 100 mg/mL (296.45 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg	
	1 mM	2.9645 mL	14.8223 mL	29.6446 mL	
	5 mM	0.5929 mL	2.9645 mL	5.9289 mL	
	10 mM	0.2964 mL	1.4822 mL	2.9645 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 (7.41 mM); Suspended solution; Need ultrasonic
- 2. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.5 mg/mL (7.41 mM); Clear solution

## **BIOLOGICAL ACTIVITY**

Description	DUB-IN-1 is an active inhibitor of ubiquitin-specific proteases (USPs), with an IC <sub>50</sub> of 0.85 $\mu$ M for USP8 <sup>[1]</sup> .				
IC <sub>50</sub> & Target	IC50: $0.24~\mu\text{M}~(\text{USP8})^{[1]}$				
In Vitro	DUBs-IN-1 (22 d) is an active inhibitor of ubiquitin-specific proteases, with an IC $_{50}$ of 0.85 $\mu$ M for USP8. DUBs-IN-1 is inactive toward USP7 (IC $_{50}$ , >100 $\mu$ M). DUBs-IN-1 and its analogs reduce the viability of HCT116 colon and PC-3 prostate cancer cell lines with IC $_{50}$ s ranging from 0.5 $\mu$ M to 1.5 $\mu$ M <sup>[1]</sup> . MCE has not independently confirmed the accuracy of these methods. They are for reference only.				

## **CUSTOMER VALIDATION**

- J Adv Res. 2022 Nov;41:1-12.
- Cell Chem Biol. 2021 Apr 27;S2451-9456(21)00213-0.
- J Med Chem. 2022 Oct 11.
- Cell Biol Toxicol. 2022 Jan 13.
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[1]. Colombo M, et al. Synthesis and biological evaluation of 9-oxo-9H-indeno[1,2-b]pyrazine-2,3-dicarbonitrile analogues as potential inhibitors of deubiquitinating enzymes. ChemMedChem. 2010 Apr 6;5(4):552-8.

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

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