**Proteins** 

# **Screening Libraries**

# SIRT-IN-1

Target:

Cat. No.: HY-16615 CAS No.: 1431411-60-7

Molecular Formula:  $C_{19}H_{27}N_5O_2S$ 389.52 Molecular Weight:

Pathway: Cell Cycle/DNA Damage; Epigenetics

Sirtuin

Storage: 4°C, protect from light

\* In solvent: -80°C, 6 months; -20°C, 1 month (protect from light)

**Product** Data Sheet

## **SOLVENT & SOLUBILITY**

In Vitro

DMSO: 19.23 mg/mL (49.37 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	2.5673 mL	12.8363 mL	25.6726 mL
	5 mM	0.5135 mL	2.5673 mL	5.1345 mL
	10 mM	0.2567 mL	1.2836 mL	2.5673 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: ≥ 1.92 mg/mL (4.93 mM); Clear solution
- 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 1.92 mg/mL (4.93 mM); Clear solution
- 3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 1.92 mg/mL (4.93 mM); Clear solution

# **BIOLOGICAL ACTIVITY**

Description SIRT-IN-1 is a potent inhibitor of SIRT1/2/3, with IC $_{50}$ s of 15, 10, 33  $\mu$ M, respectively.

IC<sub>50</sub> & Target SIRT1 SIRT2 SIRT3 15 nM (IC<sub>50</sub>) 10 nM (IC<sub>50</sub>) 33 nM (IC<sub>50</sub>)

In Vitro

SIRT-IN-1 (compound 28) is one of the most potent truncated pan SIRT1/ 2/3 inhibitor, the IC $_{50}$  values are 0.015, 0.010, 0.033 μΜ, respectively. SIRT-IN-1 (SIRT1/2/3 pan inhibitor) binds identically in the catalytic active site (RMS=0.29 Å), occupying the nicotinamide C-pocket and acetyl lysine substrate channel<sup>[1]</sup>.

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

REFERENCES				
[1]. Disch JS, et al. Discovery of thieno[3,2-d]pyrimidine-6-carboxamides as potent inhibitors of SIRT1, SIRT2, and SIRT3. J Med Chem. 2013 May 9;56(9):3666-79.				
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