**Proteins** 

# **Screening Libraries**

# **Product** Data Sheet

# DprE1-IN-2

Cat. No.: HY-100531 CAS No.: 1615713-87-5 Molecular Formula:  $C_{19}H_{24}N_6O_2$ Molecular Weight: 368.43 Target: Bacterial Pathway: Anti-infection

Storage: Powder

2 years

3 years

-80°C In solvent 2 years

-20°C

-20°C 1 year

### **SOLVENT & SOLUBILITY**

In Vitro

DMSO: ≥ 33 mg/mL (89.57 mM)

\* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	2.7142 mL	13.5711 mL	27.1422 mL
	5 mM	0.5428 mL	2.7142 mL	5.4284 mL
	10 mM	<b>0 mM</b> 0.2714 mL 1.3571	1.3571 mL	2.7142 mL

Please refer to the solubility information to select the appropriate solvent.

## **BIOLOGICAL ACTIVITY**

 $DprE1-IN-2 \ (compound\ 18) \ is\ a\ potent\ DprE1\ inhibitor\ with\ an\ IC_{50}\ of\ 28\ nM.\ DprE1-IN-2\ has\ antituberculosis\ effect^{[1]}.$ Description

IC<sub>50</sub> & Target DprE1<sup>[1]</sup>

In Vivo DprE1-IN-2 (compound 18; oral; 100 mg/kg) has  $t_{1/2}$  of 0.9 hours and  $C_{max}$  of 70  $\mu$ M in BALB/c Mice<sup>[1]</sup>.

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

Animal Model:	BALB/c Mice <sup>[1]</sup>	
Dosage:	100 mg/kg	
Administration:	Oral	
Result:	Had $t_{1/2}$ of 0.9 hours and $C_{\text{max}}$ of 70 $\mu$ M.	

REFERENCES			
[1]. Shirude PS et al. Lead optimization of 1,4-azaindoles as antimycobacterial agents. J Med Chem. 2014 Jul 10;57(13):5728-37.			
Caution: Product has not been fully validated for medical applications. For research use only.			
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