# **Product** Data Sheet

### **NBD-557**

Cat. No.: HY-76649

CAS No.: 333352-59-3

Molecular Formula: C<sub>17</sub>H<sub>24</sub>BrN<sub>3</sub>O<sub>2</sub>

Molecular Weight: 382.3 Target: HIV

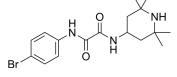
Pathway: Anti-infection

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: 10 mg/mL (26.16 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg	
	1 mM	2.6157 mL	13.0787 mL	26.1575 mL	
	5 mM	0.5231 mL	2.6157 mL	5.2315 mL	
	10 mM	0.2616 mL	1.3079 mL	2.6157 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 mg/mL (2.62 mM); Clear solution
- 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE- $\beta$ -CD in saline) Solubility:  $\geq$  1 mg/mL (2.62 mM); Clear solution

#### **BIOLOGICAL ACTIVITY**

Description

NBD-557 is a potentially HIV-1 inhibitor.IC50 Value: Target: HIVNBD-557, is small molecule organic compounds with drug-like properties. It showed potent cell fusion and virus-cell fusion inhibitory activity at low micromolar levels. A systematic study showed that NBD-557 target viral entry by inhibiting the binding of HIV-1 envelope glycoprotein gp120 to the cellular receptor CD4 but did not inhibit reverse transcriptase, integrase, or protease, indicating that they do not target the later stages of the HIV-1 life cycle to inhibit HIV-1 infection. NBD-557 potent inhibitors of both X4 and R5 viruses tested in CXCR4 and CCR5 expressing cell lines, respectively, indicating that its anti-HIV-1 activity is not dependent on the coreceptor tropism of the virus. A surface plasmon resonance study, which measures binding affinity, clearly demonstrated that NBD-557 bind to unliganded HIV-1 gp120 but not to the cellular receptor CD4. NBD-557 was active against HIV-1 laboratory-adapted strains including an AZT-resistant strain and HIV-1 primary isolates, indicating that NBD-557 can potentially be further modified to become potent HIV-1 entry inhibitors.

IC<sub>50</sub> & Target HIV-1

## **CUSTOMER VALIDATION**

• Int J Antimicrob Agents. 2019 Dec;54(6):814-819.

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REFERENCES					
REFERENCE >					

[1]. Arne Schön, et al. Thermodynamics of binding of a low-molecular-weight CD4 mimetic to HIV-1 gp120. Biochemistry. 2006 Sep 12;45(36):10973-80.

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

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