Product data sheet



MedKoo Cat#: 526801				
Name: NBD-556				
CAS: 333353-44-9 (free base)				
Chemical Formula: C ₁₇ H ₂₄ ClN ₃ O ₂				
Exact Mass: 337.1557				
Molecular Weight: 337.848				
Product supplied as:	Powder			
Purity (by HPLC):	$\geq 98\%$			
Shipping conditions	Ambient temperature			
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.			
	In solvent: -80°C 3 months; -20°C 2 weeks.			



1. Product description:

NBD-556 is a HIV-1 entry inhibitor. NBD-556 inhibited cell–cell fusion between H9/HIV-1IIIB and MT-2 (IC50 \sim 3 μ M). NBD-556 prevent gp120 binding to CD4. The HIV-1 entry into host cells is a complex, multi-factors involved, and multi-step process. Especially, the attachment of HIV-1 envelope glycoprotein gp120 to the host cell receptor CD4 is the first key step during entry process, representing a promising antiviral therapeutic target.

2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMF	30.0	8.80
DMSO	43.78	129.58
DMSO:PBS (pH 7.2)	0.5	1.48
(1:1)		
Ethanol	6.5	19.24

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.96 mL	14.80 mL	29.60 mL
5 mM	0.59 mL	2.96 mL	5.92 mL
10 mM	0.30 mL	1.48 mL	2.96 mL
50 mM	0.06 mL	0.30 mL	0.59 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study

In vitro study

1. Yoshimura K, Harada S, Shibata J, Hatada M, Yamada Y, Ochiai C, Tamamura H, Matsushita S. Enhanced exposure of human immunodeficiency virus type 1 primary isolate neutralization epitopes through binding of CD4 mimetic compounds. J Virol. 2010 Aug;84(15):7558-68. doi: 10.1128/JVI.00227-10. Epub 2010 May 26. PMID: 20504942; PMCID: PMC2897603.

2. Schön A, Madani N, Klein JC, Hubicki A, Ng D, Yang X, Smith AB 3rd, Sodroski J, Freire E. Thermodynamics of binding of a low-molecular-weight CD4 mimetic to HIV-1 gp120. Biochemistry. 2006 Sep 12;45(36):10973-80. doi: 10.1021/bi061193r. PMID: 16953583; PMCID: PMC2504686.

In vivo study

TBD

Product data sheet



7. Bioactivity

Biological target:

NBD-556, a CD4 mimetic, is a potent HIV-1 entry inhibitor that blocks the gp120-CD4 interaction.

In vitro activity

NBD-556, like CD4, activates the binding of gp120 to the HIV-1 coreceptor, CCR5, and to the 17b monoclonal antibody, which recognizes the coreceptor binding site of gp120. NBD-556 stimulates HIV-1 infection of CD4-negative, CCR5-expressing cells. NBD-556 is a competitive inhibitor of sCD4 and elicits a similar structuring of the coreceptor binding site, whereas BMS-378806 does not compete with sCD4 and does not induce coreceptor binding.

Reference: Biochemistry. 2006 Sep 12;45(36):10973-80. https://pubmed.ncbi.nlm.nih.gov/16953583/

In vivo activity

TBD

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.