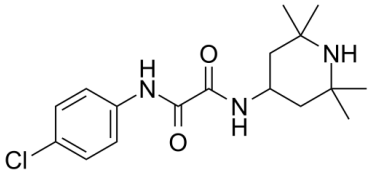
Data Sheet

Product Name:	NBD-556
Cat. No.:	CS-0526
CAS No.:	333353-44-9
Molecular Formula:	C17H24ClN3O2
Molecular Weight:	337.84
Target:	HIV
Pathway:	Anti-infection
Solubility:	H2O : < 0.1 mg/mL (insoluble); DMSO : 33.33 mg/mL (98.66 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

NBD-556 is small molecule mimetic of CD4, NBD-556 recognizes the HIV-1 envelope protein gp120 and induces restructuring of gp120 analogous to CD4 binding. IC50 Value: Target: HIV NBD-556 N-phenyl-N′-(2,2,6,6-tetramethyl-piperidin-4-yl)-oxalamide analogs as a novel class of human immunodeficiency virus type 1 (HIV-1) entry inhibitors that block the gp120–CD4 interaction. Human immunodeficiency virus (HIV-1) interaction with the primary receptor, CD4, induces conformational changes in the viral envelope glycoproteins that allow binding to the CCR5 second receptor and virus entry into the host cell. The small molecule NBD-556 mimics CD4 by binding the gp120 exterior envelope glycoprotein, moderately inhibiting virus entry into CD4-expressing target cells and enhancing CCR5 binding and virus entry into CCR5-expressing cells lacking CD4.

PROTOCOL (Extracted from published papers and Only for reference)

Cell assay [2] Cf2Th-CCR5 target cells were seeded at a density of 6 × 103 cells/well in 96-well luminometer-compatible tissue culture plates 24 h before infection. On the day of infection, NBD-556 (0-100 μM) was incubated with recombinant viruses (10,000 RT units) at 37°C for 30 min. The mixtures were then added to the target cells and incubated for 48 h at 37°C; after this time, the medium was removed from each well, and the cells were lysed by the addition of 30 μL passive lysis buffer and three freeze-thaw cycles. An EG&G Berthold Microplate Luminometer LB 96V was used to measure the luciferase activity of each well after the addition of 100 μL of luciferin buffer (15 mM MgSO4, 15 mM KPO4, pH 7.8, 1 mM ATP, and 1 mM dithiothreitol) and 50 μL of 1 mM D-luciferin potassium salt.

References:

[1]. Narumi, Tetsuo et al. CD4 mimics targeting the HIV entry mechanism and their hybrid molecules with a CXCR4 antagonist. Bioorganic & Medicinal Chemistry Letters (2010), 20(19), 5853-5858.

[2]. Schon A, et al. Thermodynamics of binding of a low-molecular-weight CD4 mimetic to HIV-1 gp120. Biochemistry. 2006 Sep 12;45(36):10973-10980.

[3]. Singh IP, Chauthe SK. Small molecule HIV entry inhibitors: Part II. Attachment and fusion inhibitors: 2004-2010. Expert Opin Ther Pat. 2011 Mar;21(3):399-416.

[4]. Zhao Q, Ma L, Jiang S, Lu H, Liu S, He Y, Strick N, Neamati N, Debnath AK. Identification of N-phenyl-N'-(2,2,6,6-tetramethyl-piperidin-4-yl)-oxalamides as a new class of HIV-1 entry inhibitors that prevent gp120 binding to CD4. Virology. 2005 Sep 1;339(2):213-25.

CAIndexNames:

Ethanediamide, N1-(4-chlorophenyl)-N2-(2,2,6,6-tetramethyl-4-piperidinyl)-

SMILES:

O=C(C(NC1CC(C)(NC(C)(C1)C)C)=O)NC2=CC=C(C=C2)Cl

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

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