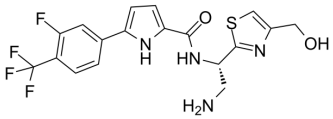
NBD-14189

Cat. No.:	HY-139985
CAS No.:	2234273-72-2
Molecular Formula:	$C_{18}H_{16}F_4N_4O_2S$
Molecular Weight:	428.4
Target:	HIV
Pathway:	Anti-infection
Storage:	4°C, sealed storage, away from moisture and light * In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture and light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (233.43 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.3343 mL	11.6713 mL	23.3427 mL
	5 mM	0.4669 mL	2.3343 mL	4.6685 mL
	10 mM	0.2334 mL	1.1671 mL	2.3343 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (5.84 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (5.84 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

NBD-14189 is a potent HIV-1 entry antagonist with an IC_{50} of 89 nM against the HIV-1_{HXB2} pseudovirus. NBD-14189 binds to HIV-1 gp120 and shows potent antiviral activity (EC_{50}<200 nM)[1][2].

IC_{50} & Target

HIV-1

In Vitro

NBD-14189 has anti-HIV-1 activity (IC_{50}=0.089 μM) and cytotoxicity (CC_{50}=21.9 μM) in single-cycle (TZM-bl cells) assays. NBD-14189 has anti-HIV-1 activity (IC_{50}=0.18 μM) and cytotoxicity (CC_{50}=22.1 μM) in multi-cycle (MT-2 cells) assays[1].

NBD-14189 (0-50 μM) prevents HIV-1 mediated cell-cell fusion with an IC_{50} of 9.4 μM in indicator cells TZM-bl cells were cocultured with Env- and Tat-expressing HL2/3 cells[1].

NBD-14189 shows weak or no inhibition of the hERG current, with an IC_{50} of 3.0 μM, respectively[1].

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

REFERENCES

[1]. Francesca Curreli, et al. Structure-based lead optimization to improve antiviral potency and ADMET properties of phenyl-1H-pyrrole-carboxamide entry inhibitors targeted to HIV-1 gp120. Eur J Med Chem. 2018 Jun 25;154:367-391.

[2]. Natalie Losada, et al. HIV-1 gp120 Antagonists Also Inhibit HIV-1 Reverse Transcriptase by Bridging the NNRTI and NRTI Sites. J Med Chem. 2021 Nov 25;64(22):16530-16540.

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