

NNRT-IN-10

Chemical Properties

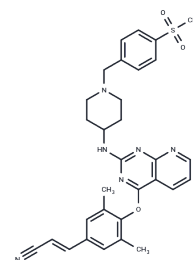
CAS No. : 2459751-62-1

Formula: C₃₁H₃₂N₆O₃S

Molecular Weight: 568.69

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Actual storage temperature shall be subject to the COA.



Biological Description

| | |
|----------------------------|--|
| Description | NNRT-IN-10 is a potent, selective, and orally bioavailable non-nucleoside reverse transcriptase inhibitor (NNRTI) for HIV-1. The compound exhibits EC ₅₀ values ranging from 1.16 to 18.3 nM against HIV and its variants. NNRT-IN-10 has favorable pharmacokinetic properties and safety profile, making it suitable for research on AIDS caused by HIV-1. |
| Targets(IC ₅₀) | HIV Protease,Reverse Transcriptase,Cytochromes P450,Potassium Channel |
| In vitro | NNRT-IN-10 (Compound 5i3) demonstrates improved resistance profiles and negligible cytotoxicity, with EC ₅₀ values of 1.16 nM for HIV-1 (WT), 2.64 nM for P1579, 12.5 nM for P5375, 3.70 nM for P1833, and 18.3 nM for P5735. In MT-4 cells over five days, NNRT-IN-10 effectively inhibits HIV-1 IIIB replication at nanomolar levels (EC ₅₀ = 1.4 nM). It exhibits weak inhibition against cytochrome P450 enzymes: CYP1A2 (IC ₅₀ = 56.6 μM), CYP2C9 (IC ₅₀ = 6.76 μM), CYP2C19 (IC ₅₀ = 8.47 μM), and CYP2D6 (IC ₅₀ = 12.7 μM). Additionally, NNRT-IN-10 demonstrates potassium channel inhibitory activity in CHO-hERG cells (0.3-40 μM, 24 h), with an IC ₅₀ of 1.48 μM. |
| In vivo | NNRT-IN-10 (Compound 5i3) is well-tolerated at a single oral dose of 800 mg/kg, exhibiting no acute toxicity in mice. |

Preparing Stock Solutions

| | 1mg | 5mg | 10mg |
|-------|------------|------------|-------------|
| 1 mM | 1.7584 mL | 8.7921 mL | 17.5843 mL |
| 5 mM | 0.3517 mL | 1.7584 mL | 3.5169 mL |
| 10 mM | 0.1758 mL | 0.8792 mL | 1.7584 mL |
| 50 mM | 0.0352 mL | 0.1758 mL | 0.3517 mL |

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

This product is for Research Use Only · Not for Human or Veterinary or Therapeutic Use

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