# Product Datasheet

## Technical Data

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| **Formula** | $C_{20}H_{19}F_2N_3O_5$ | | | | | |
| **Molecular Weight** | 419.38 | **CAS No.** | 1051375-16-6 | | | |
| **Solubility (25°C)*** | In vitro | DMSO | 84 mg/mL (200.29 mM) | | | |
| | | Water | Insoluble | | | |
| | | Ethanol | Insoluble | | | |
| | *In vivo* (Add solvents to the product individually and in order) | Oral Administration | Homogeneous suspension | CMC-NA | ≥5mg/ml | Taking the 1 mL working solution as an example, add 5 mg of this product to 1 ml of CMC-Na solution, mix evenly to obtain a homogeneous suspension with a final concentration of 5 mg/ml. |

* <1 mg/ml means slightly soluble or insoluble.
* Please note that Capsid Bio tests the solubility of all compounds in-house, and the actual solubility may differ slightly from published values. This is normal and is due to slight batch-to-batch variations.
* Room temperature shipping (Stability testing shows this product can be shipped at 2-8°C for storage purposes.)

## Preparing Stock Solutions

## Biological Activity

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| **Description** | Dolutegravir is a two-metal-binding HIV **integrase** inhibitor with **IC50** of 2.7 nM in a cell-free assay, modest activity against raltegravir-resistant signature mutants Y143R, Q148K, N155H, and G140S/Q148H. |
| **Targets** | HIV integrase [2]<br>(Cell-free assay)<br>2.7 nM |
| **In vitro** | Dolutegravir (GSK1349572) shows a potent inhibitory effect on nine clinical isolates from integrase inhibitor-naive HIV-2-infected patients with EC50 ranging from 0.2 nM to 1.4 nM.[1]<br>In vitro, it inhibits recombinant HIV-1 integrase-catalyzed strand transfer with an IC50 of 2.7 nM. Furthermore, this compound potently inhibits HIV replication in cells such as peripheral blood mononuclear cells (PBMCs), MT-4 cells, and CIP4 cells infected with a self-inactivating PHIV lentiviral vector, with EC50 values of 0.51 nM, 0.71 nM, and 2.2 nM, respectively.[2]<br>In vitro, it also exhibits potent activity against five different nonnucleoside reverse transcription inhibitor-resistant or nucleoside reverse transcription inhibitor-resistant viruses, with EC50 ranging from 1.3 nM to 2.1 nM. Similarly to its activity against wild-type virus, it shows equivalent efficacy against two protease inhibitor-resistant viruses, with EC50 values of 0.36 nM and 0.37 nM, respectively.[2] |
| **In vivo** | Dolutegravir (GSK1349572), a first-line antiretroviral drug (ARV) used in combination therapy for HIV-1, inhibits MMP activity and has the potential to affect prenatal and postnatal neurodevelopment. |
| **Features** | A next-generation and two-metal-binding HIV integrase strand transfer inhibitor. |

## Protocol (from reference)

**Kinase Assay:**[2]

- **In vitro strand transfer assay**

  The inhibitory potencies of Dolutegravir (GSK1349572) and other INIs are measured in a strand transfer assay using recombinant HIV integrase. A complex of integrase and biotinylated preprocessed donor DNA-streptavidin-coated scintillation proximity assay (SPA) beads is formed by incubating 2 μM purified recombinant integrase with 0.66 μM biotinylated donor DNA-4 mg/mL streptavidin-coated SPA beads in 25 mM sodium morpholinepropanesulfonic acid (MOPS) (pH 7.2), 23 mM NaCl, and 10 mM $MgCl_2$ for 5 minutes at 37 °C. These beads are spun down and preincubated with diluted INIs for 60 minutes at 37 °C. Then a $_3$H-labeled target DNA substrate is added to give a final concentration of 7 nM substrate, and the strand transfer reaction mixture is incubated at 37 °C for 25 to 45 minutes, which allows for a linear increase in the strand transfer of donor DNA to radiolabeled target DNA. The signal is read using a Wallac MicroBeta scintillation plate reader.

**Cell Assay:**[2]

- **Cell lines**

  MT-4
- **Concentrations**

  0 to 10 μM
- **Incubation Time**

  4 days or 5 days
- **Method**

  Exponentially growing MT-4 cells at a density of 500,000 or 600,000/mL are infected with HIV-1 strain IIIB at a viral multiplicity of infection of 0.001 or a 50% tissue culture infective dose of 4 to 10. The cells are then aliquoted to 96-well plates in the presence of varying concentrations of Dolutegravir (GSK1349572). After incubation for 4 or 5 days, antiviral activity is determined by a cell viability assay that either measured bioluminescence with a CellTiter-Glo luminescent reagent or measured absorbance at 560 and 690 nm using the yellow tetrazolium MTT reagent [3-(4,5-dimethyl-2-thiazolyl)-2,5-diphenyltetrazolium bromide].

**Animal Study:**[3]

- **Animal Models**

  C3H/HeJ mice
- **Dosages**

  50 mg/kg
- **Administration**

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## References


https://pubmed.ncbi.nlm.nih.gov/20827161/ https://pubmed.ncbi.nlm.nih.gov/21115794/ https://pubmed.ncbi.nlm.nih.gov/34390469/


### RETURN POLICY

Capsid Bio's Unconditional Return Policy ensures a smooth online shopping experience for our customers. If you are in any way unsatisfied with your purchase, you may return any item(s) within 7 days of receiving it. In the event of product quality issues, either protocol related or product related problems, you may return any item(s) within 365 days from the original purchase date. Please follow the instructions below when returning products.

### SHIPPING & STORAGE

Capsid Bio products are transported at room temperature. If you receive the product at room temperature, please rest assured, the Capsid Bio Quality Inspection Department has conducted experiments to verify that the normal temperature placement of one month will not affect the biological activity of powder products. After collecting, please store the product according to the requirements described in the datasheet. Most Capsid Bio products are stable under the recommended conditions.

**NOT FOR HUMAN, VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.**


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