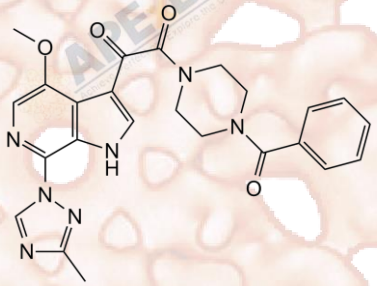
Product Data Sheet

# BMS-626529



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| **Cat. No.:** | A3253 |
| **CAS No.:** | 701213-36-7 |
| **Formula:** | C24H23N7O4 |
| **M.Wt:** | 473.48 |
| **Synonyms:** | BMS 626529;BMS626529 |
| **Target:** | Proteases |
| **Pathway:** | HIV Protease |
| **Storage:** | Store at -20°C |

## Solvent & Solubility

In Vitro

insoluble in H2O; insoluble in EtOH; ⩾1.48 mg/mL in DMSO

Preparing Stock Solutions

| Mass / Solvent / Concentration | 1mg | 5mg | 10mg |
|---|---|---|---|
| **1 mM** | 2.1120 mL | 10.5601 mL | 21.1202 mL |
| **5 mM** | 0.4224 mL | 2.1120 mL | 4.2240 mL |
| **10 mM** | 0.2112 mL | 1.0560 mL | 2.1120 mL |

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

## Biological Activity

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|---|---|
| Shortsummary | HIV-1 attachment inhibitor |
| $IC_{50}$ & Target | 2.26 nM (HIV-1 subtype A envelope), 0.34 nM (HIV-1 subtype B envelope), 1.3 nM (HIV-1 subtype C envelope) |

In Vitro

**Cell Viability Assay**

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| Cell Line: | PBMCs infected with HIV-1 clinical isolates; MT-2 and PM1 cells |
| Preparation method： | Soluble in DMSO. General tips for obtaining a higher concentration: Please warm the tube at 37°C for 10 minutes and/or shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months. |
| Reacting conditions: | 6 days; dissolved in 100% dimethyl sulfoxide (DMSO) and serially diluted to the |

| | | |
|---|---|---|
| | | desired concentration such that the final DMSO concentration in cell culture assays was 1%. |
| | Applications: | BMS-626529 exhibits low cytotoxicity in several cell types from different human tissues such as MT-2 (T lymphocytes), HEK293 (kidney), PM1 and PBMCs. BMS-626529 exhibits EC50 value against the CXCR4-tropic LAI virus of 0.7 nM and also exhibits broad spectrum of activity. |
| In Vivo | **Animal experiment** | |
| | Dosage form: | 600 mg or 1200mg with or without 100 mg ritonavir; 8 days; orally administrated. |
| | Applications: | BMS-663068, the prodrug of BMS-626529, reduces plasma HIV-1 RNA levels and increases median absolute CD4+ T-cell counts. Also, BMS-663068 is well tolerated. BMS-626529 has favorable pharmacokinetics following administration of the prodrug BMS-663068. |
| | Other notes: | Please test the solubility of all compounds indoor, and the actual solubility may slightly differ with the theoretical value. This is caused by an experimental system error and it is normal. |

## Product Citations

1. Stadtmueller BM, Bridges MD, et al. "DEER Spectroscopy Measurements Reveal Multiple Conformations ofHIV-1 SOSIP Envelopes that Show Similarities with Envelopes on Native Virions."Immunity. 2018 Aug 21;49(2):235-246.e4.PMID:30076100
2. Pancera M, Lai YT, et al. "Crystal structures of trimeric HIV envelope with entry inhibitors BMS-378806 and BMS-626529." Nat Chem Biol. 2017 Oct;13(10):1115-1122.PMID:28825711

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## References

[1]. Nowicka-Sans B, Gong YF, McAuliffe B, et al. In vitro antiviral characteristics of HIV-1 attachment inhibitor BMS-626529, the active component of the prodrug BMS-663068. Antimicrob Agents Chemother, 2012, 56(7): 3498-3507.
[2]. Nettles RE, Schürmann D, Zhu L, et al. Pharmacodynamics, safety, and pharmacokinetics of BMS-663068, an oral HIV-1 attachment inhibitor in HIV-1-infected subjects. J Infect Dis, 2012, 206(7): 1002-1011.

## Caution

**FOR RESEARCH PURPOSES ONLY.**

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

*Specific storage and handling information for each product is indicated on the product datasheet. Most APExBIO products are stable under the recommended conditions. Products are sometimes shipped at a temperature that differs from the recommended storage temperature. Shortterm storage of many products are stable in the short-term at temperatures that differ from that required for long-term storage. We ensure that the product is shipped under conditions that will maintain the quality of the reagents. Upon receipt*

*of the product, follow the storage recommendations on the product data sheet.*

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