# Temsavir

**Cat. No.:** HY-15440

**CAS No.:** 701213-36-7

**Molecular Formula:** $C_{24}H_{23}N_7O_4$

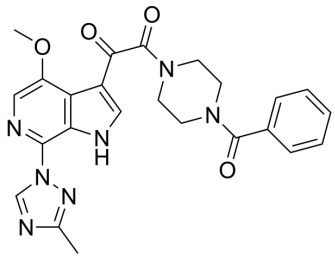
**Molecular Weight:** 473.48

**Target:** HIV

**Pathway:** Anti-infection

**Storage:**

| | | |
|---|---|---|
| Powder | -20°C | 3 years |
| | 4°C | 2 years |
| In solvent | -80°C | 2 years |
| | -20°C | 1 year |



## SOLVENT & SOLUBILITY

**In Vitro**

DMSO : ≥ 16.67 mg/mL (35.21 mM)

* "≥" means soluble, but saturation unknown.

**Preparing Stock Solutions**

| Solvent / Mass / Concentration | 1 mg | 5 mg | 10 mg |
|---|---|---|---|
| 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.

**In Vivo**

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 1.67 mg/mL (3.53 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 1.67 mg/mL (3.53 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 1.67 mg/mL (3.53 mM); Clear solution

## BIOLOGICAL ACTIVITY

**Description**

Temsavir (BMS-626529) is a novel attachment inhibitor that targets HIV-1 gp120 and prevents its binding to $CD4^+$ T cells.

**$IC_{50}$ & Target**

HIV-1

**In Vitro**

Temsavir has half-maximal effective concentration ($EC_{50}$) values of <10 nM against the vast majority of viral isolates. Temsavir exhibits an average $EC_{50}$ against LAI virus of 0.7±0.4 nM. Temsavir exhibits an $EC_{50}$ of 0.01 nM against the most

susceptible virus and an $EC_{50}$ of >2,000 nM against the least susceptible virus. The cytotoxicity profile of Temsavir is examined in several cell types from different human tissues. $CC_{50}$ values of >200 μM are observed in MT-2 (T lymphocytes), HEK293 (kidney), HEp-2 (larynx), HepG2 (liver), HeLa (cervix), HCT116 (colorectal), MCF-7 (breast), SK-N-MC (neuroepithelium), HOS (bone), H292 (lung), and MDBK (bovine kidney) cells measured after 3 or 6 days in culture. $CC_{50}$ values of 105 and 192 μM are obtained in the T-cell line PM1 and in PBMCs, respectively, following 6 days in culture. These results show that Temsavir exhibits low cytotoxicity in cell culture[1]. Temsavir exhibits a broad spectrum of antiviral activity against a panel of clinical isolates, with a 50% inhibitory concentration ($IC_{50}$) ranging from subnanomolar levels to >0.1 μM [2].

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

## PROTOCOL

**Kinase Assay** [1]

Micro BioSpin 6 columns are used to measure the binding of [$^3$H]BMS-488043 or [$^3$H]Temsavir to gp120. Binding solutions (30 μL) containing 25 mM Tris-HCl (pH 7.5), 125 mM NaCl, 50 nM $gp120_{JRFL}$, and serial dilutions of [$^3$H]BMS-488043 or [$^3$H]Temsavir are allowed to equilibrate and then adsorbed to a MicroBioSpin 6 column. The column is centrifuged (~14,000 rpm) for 5 min, the eluent is collected, and radioactivity is determined with a scintillation counter. To measure dissociative kinetics, 150 nM [$^3$H]Temsavir or 90 nM [$^3$H]BMS-488043 is incubated with 60 nM gp120 at ambient temperature for 1 h to achieve equilibrium binding, and then a large molar excess (14-fold) of soluble CD4 protein is added to drive dissociation. Aliquots are taken at the indicated time intervals, adsorbed to a spin column, and centrifuged, and the radioactivity in the eluent is quantitated. Comparison of the tritium signal from parallel samples with and without the soluble CD4 challenge allowed for the determination of the percent compound bound[1].

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**Cell Assay** [1]

Cytotoxicity assays are performed in the presence of serially diluted Temsavir for up to 6 days, and cell viability is quantitated using an XTT assay. To determine $CC_{50}$ values (concentration of drug required to kill 50% of cells), laboratory-adapted peripheral blood mononuclear cells (PBMCs) are initially plated at a density of $0.1\times10^6$ cells/mL. In the absence of compounds, the cell densities typically reach $1\times10^6$ to $1.2\times10^6$/mL after 6 days[1].

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## CUSTOMER VALIDATION

- Commun Biol. 2021 Jan 20;4(1):93.
- J Antimicrob Chemother. 2021 Aug 17;dkab309.
- J Antimicrob Chemother. 2020 Sep 1;75(9):2547-2553.
- Molecules. 2020 Mar 21;25(6):1430.

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## REFERENCES

[1]. Nowicka-Sans B, et al. In vitro antiviral characteristics of HIV-1 attachment inhibitor BMS-626529, the active component of the prodrug BMS-663068. Antimicrobial Agents and Chemotherapy (2012), 56(7), 3498-3507.

[2]. Nettles RE, et al. Pharmacodynamics, safety, and pharmacokinetics of BMS-663068, an oral HIV-1 attachment inhibitor in HIV-1-infected subjects. J Infect Dis. 2012 Oct 1;206(7):1002-11.

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

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