

Product Data Sheet

Product Name: BMS-663068

Cat. No.: GC13119

Chemical Properties

Cas. No. 864953-29-7

Chemical Name (3-(2-(4-benzoylpiperazin-1-yl)-2-oxoacetyl)-4-methoxy-7-(3-methyl-1H-1,2,4-triazol-1-yl)-1H-pyrrolo[2,3-c]pyridin-1-yl)methyl dihydrogen phosphate

SMILES CC1=NN(C2=NC=C(OC)C3=C2N(COP(O)(O)=O)C=C3C(C(N4CCN(C(C5=CC=CC=C5)=O)CC4)=O)=O)C=N1

Formula $C_{25}H_{26}N_7O_8P$ M.Wt 583.49

Solubility DMSO : 100mg/mL Storage Store at -20°C

General tips For obtaining a higher solubility , please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.

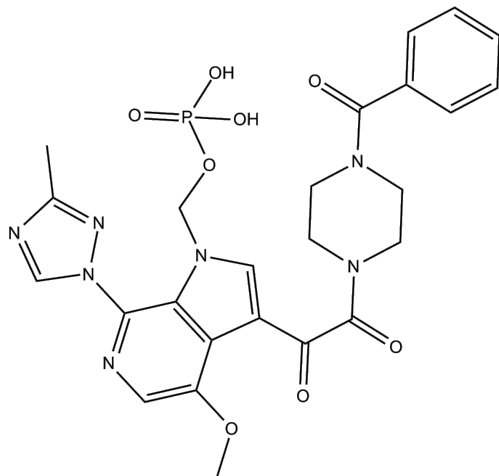
Caution: Product has not been fully validated for medical applications. For research use only.

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Structure



Background

BMS-663068 is a small-molecule attachment inhibitor of HIV-1 gp120 with IC₅₀ value of [1]. The first step of HIV-1 virus to entry host cells is the binding of the viral gp120 envelope glycopeptide to the CD4 receptor of host cell. BMS-663068 is an attachment inhibitor against specific HIV-1 isolates and targets this step. It is a phosphonoxy methyl prodrug and can be cleaved by alkaline phosphatase in the gut then releases the effective moiety BMS-626529. Compared with the progenitor attachment inhibitor BMS-488043, BMS-663068 has an improved antiviral spectrum [1]. BMS-663068 showed low cytotoxicity in cell culture. In PM1 and PBMC cells, the CC₅₀ values were 105 and 192 μ M, respectively. In HEK293, HepG2, HCT116, HeLa, MT-2, MCF-7 and H292 cells, the CC₅₀ values were all higher than 200 μ M. It was found that BMS-663068 has potent anti-virus activity against both the laboratory strains and the clinical isolates of HIV. For the CXCR4-tropic LAI virus, BMS-663068 showed EC₅₀ value of 0.7 nM. For a cohort of laboratory strains including NL4-3, SF-162 and JRFL, the inhibition efficacies of BMS-663068 against them were 7 to 10-fold higher than that of BMS-488043. It was even more potent than BMS-488043 when treated with 89.6 viruses (15-fold), Bal virus (14-fold) and MN virus (67-fold). In an antiviral assay using PBMC cells, BMS-663068

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was treated against a total of 88 HIV-1 viruses obtained from the NIH AIDS Repository. It exerted an EC₅₀ value of 0.01 nM against the most susceptible virus and an EC₅₀ value of 2μM against the least susceptible virus. In addition, it was found that the virus resistant to other HIV-1 entry inhibitors such as ENF and ibalizumab retained susceptibility to BMS-626529 [1 and 2].

References:

[1] Nowicka-Sans B, Gong YF, McAuliffe B, Dicker I, Ho HT, Zhou N, Eggers B, Lin PF, Ray N, Wind-Rotolo M, Zhu L, Majumdar A, Stock D, Lataillade M, Hanna GJ, Matiskella JD, Ueda Y, Wang T, Kadow JF, Meanwell NA, Krystal M. *In vitro* antiviral characteristics of HIV-1 attachment inhibitor BMS-626529, the active component of the prodrug BMS-663068. *Antimicrob Agents Chemother.* 2012 Jul;56(7):3498-507.

[2] Li Z, Zhou N, Sun Y, Ray N, Lataillade M, Hanna GJ, Krystal M. Activity of the HIV-1 attachment inhibitor BMS-626529, the active component of the prodrug BMS-663068, against CD4-independent viruses and HIV-1 envelopes resistant to other entry inhibitors. *Antimicrob Agents Chemother.* 2013 Sep;57(9):4172-80.

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