Chemical Properties

Product Name: BMS-663068

Cas No.: 864953-29-7

M.Wt: 583.49

Formula: C25H26N7O8P

Synonyms: BMS663068; BMS 663068

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

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

Solubility: DMSO

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.

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

Biological Activity

Targets: gp120/CD4

Pathways: Microbiology & Virology >> gp120/CD4

Description:

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 phosphonooxy 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 antivirus spectrum [1]. BMS-663068 showed low cytotoxicity in cell culture. In PM1 and PBMC cells, the CC50 values were 105 and 192 μM, respectively. In HEK293, HepG2, HCT116, HeLa, MT-2, MCF-7 and H292 cells, the CC50 values were all higher than 200 μM. 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 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].

Reference:

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.