Product Data Sheet

Chemical Properties

Product Name: Asunaprevir (BMS-650032)
Cas No.: 630420-16-5
M.Wt: 748.29
Formula: C35H46ClN5O9S
Synonyms: BMS-650032; BMS 650032; BMS650032, Asunaprevir
Chemical Name: tert-butyl N-[(2S)-1-[(2S,4R)-4-(7-chloro-4-methoxyisooquinolin-1-yl)oxy-2-[[[(1R,2S)-1-(cyclopropylsulfonyl)carbamoyl]-2-ethenylcyclopropyl]carbamoyl[pyrroloidin-1-yl]-3,3-dimethyl-1-oxobutan-2-yl]carbamate
Canonical SMILES: CC(C)(C(C(=O)N1CC(CC1C(=O)NC2(CC2C=C(C(=O)NS(=O)(=O)C3CC3)OC4=NC=C(C5=C4C=CC=C(C=C5)Cl)OC)NC(=O)OC(C(C)C
Solubility: >37.4mg/mL in 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: HCV Protease
Pathways: Proteases >> HCV Protease
Description: Asunaprevir is an orally efficacious inhibitor of NS3 protease with IC50 value of 1nM [1].
Asunaprevir is an inhibitor of hepatitis C virus (HCV) NS3 protease. It can inhibit 6 major genotypes of HCV NS3/4A protease with IC50 values of 0.7nM, 0.3nM, 15nM, 78nM, 320nM, 1.6nM, 1.7nM and 0.9nM, respectively for genotype 1a, 1b, 2a, 2b, 3a, 4a, 5a and 6a, respectively. When using the purified recombinant full-length HCV NS3/4A protease complexes, asunaprevir shows the Ki values of 0.4nM and 0.2nM, respectively for genotype 1a and genotype 1b. The mechanism of the inhibition is that the acylsulfonamide of asunaprevir interacts with the catalytic site of NS3 protease in a noncovalent manner. Asunaprevir inhibits HCV RNA replication in different cell lines, including liver, T lymphocytes, lung, cervix, and embryonic kidney. It shows no obvious activity against other RNA viruses. The permeability of asunaprevir is similar to the compound with good absorption in humans. The tests of metabolism rate show that asunaprevir exhibits low to intermediate metabolic clearance. Plasma and tissue exposures in vivo indicate that asunaprevir displays a hepatotropic disposition [2].

Reference:


Protocol

Cell experiment:

Cell lines
HuH-7, MRC5, MT-2, HepG2, HeLa and HEK293 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
4 days

Applications
Asunaprevir inhibited HCV RNA replication in different cell lines, including liver, T lymphocytes, lung, cervix, and embryonic kidney. It showed no obvious activity against other RNA viruses.

Animal experiment [3]:


Animal models: Rats
Dosage form: 10 μM; p.o.; 60 mins
Applications: After oral dosing to the rat, Asunaprevir demonstrated modest oral bioavailability and a plasma AUC of 1.0 μM·h. However, at the 24th hrs after p.o. dosing, the liver levels of Asunaprevir were high at 15.2 μM, suggesting a hepatotropic distribution in vivo.

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.

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. Short-term 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.