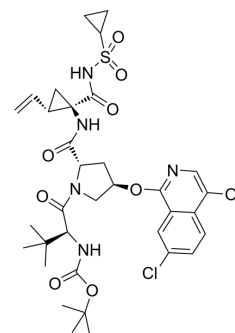


## Asunaprevir

<b>Cat. No.:</b>	HY-14434		
<b>CAS No.:</b>	630420-16-5		
<b>Molecular Formula:</b>	C <sub>35</sub> H <sub>46</sub> ClN <sub>5</sub> O <sub>9</sub> S		
<b>Molecular Weight:</b>	748.29		
<b>Target:</b>	HCV; HCV Protease; SARS-CoV		
<b>Pathway:</b>	Anti-infection; Metabolic Enzyme/Protease		
<b>Storage:</b>	Powder	-20°C	3 years
		4°C	2 years
	In solvent	-80°C	2 years
		-20°C	1 year



### SOLVENT & SOLUBILITY

#### In Vitro

DMSO : ≥ 100 mg/mL (133.64 mM)  
 Ethanol : 20 mg/mL (26.73 mM; Need ultrasonic)  
 \* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Solvent Concentration	Mass		
		1 mg	5 mg	10 mg
	1 mM	1.3364 mL	6.6819 mL	13.3638 mL
	5 mM	0.2673 mL	1.3364 mL	2.6728 mL
	10 mM	0.1336 mL	0.6682 mL	1.3364 mL

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

#### In Vivo

- Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline  
Solubility: ≥ 2.5 mg/mL (3.34 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)  
Solubility: ≥ 2.5 mg/mL (3.34 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% corn oil  
Solubility: ≥ 2.5 mg/mL (3.34 mM); Clear solution
- Add each solvent one by one: 5% DMSO >> 40% PEG300 >> 5% Tween-80 >> 50% saline  
Solubility: 2.5 mg/mL (3.34 mM); Suspended solution; Need ultrasonic
- Add each solvent one by one: 10% EtOH >> 40% PEG300 >> 5% Tween-80 >> 45% saline  
Solubility: 2 mg/mL (2.67 mM); Clear solution; Need ultrasonic
- Add each solvent one by one: 10% EtOH >> 90% corn oil  
Solubility: ≥ 2 mg/mL (2.67 mM); Clear solution

### BIOLOGICAL ACTIVITY

<b>Description</b>	Asunaprevir (BMS-650032) is a potent and orally bioavailable hepatitis C virus (HCV) NS3 protease inhibitor, with IC <sub>50</sub> of 0.2 nM-3.5 nM <sup>[1]</sup> . Asunaprevir inhibits SARS-CoV-2 3CL <sup>Pro</sup> activity <sup>[5]</sup> .
<b>IC<sub>50</sub> &amp; Target</b>	IC <sub>50</sub> : 0.2 nM-3.5 nM (HCV NS3 protease)
<b>In Vitro</b>	In multiple experiments, populations of resistant colonies are markedly reduced when cells are treated with a combination of DCV and Asunaprevir <sup>[1]</sup> . Asunaprevir (ASV) inhibits the NS3 proteolytic activity of genotype 1a (H77 strain) and genotype 1b (J4L6S strain), with IC <sub>50</sub> s of 0.7 and 0.3 nM, respectively. The EC <sub>50</sub> s of ASV against replicons encoding the NS3 protease domains representing genotypes 1a, 1b, and 4a, range from 1.2 to 4.0 nM <sup>[2]</sup> . Replicon cells are maintained under selective pressure with asunaprevir at concentrations of 10 and 30 times the EC <sub>50</sub> values (50 or 150 nM final concentrations, respectively). For genotype 1b resistance selection, replicon cells are maintained in the presence of asunaprevir at 10 or 30 times the EC <sub>50</sub> values (30 or 90 nM final concentrations, respectively) <sup>[3]</sup> . MCE has not independently confirmed the accuracy of these methods. They are for reference only.
<b>In Vivo</b>	Asunaprevir (ASV, 3-15 mg/kg, p.o.) displays a hepatotropic disposition (liver-to-plasma ratios ranging from 40- to 359-fold across species) in several animal species. Twenty-four hours postdose, liver exposures across all species tested are ≥110-fold above the inhibitor EC <sub>50</sub> observed with HCV genotype-1 replicons <sup>[2]</sup> . MCE has not independently confirmed the accuracy of these methods. They are for reference only.

## PROTOCOL

<b>Cell Assay</b> <sup>[2]</sup>	Cytotoxicity is determined by incubating cells (3,000 to 10,000 cells/well) with serially diluted test compounds or DMSO for 5 days (MT-2 cells) or 4 days (all other cell types). Cell viability is quantitated using an MTS assay for MT-2 or a Cell-Titer Blue reagent assay for HEK-293, HuH-7, HepG2, and MRC5 cells, and 50% cytotoxic concentrations (CC <sub>50</sub> s) are calculated. For the HCV and BVDV replicon assays, CC <sub>50</sub> s are determined from the same wells that are later used to determine EC <sub>50</sub> s. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
<b>Animal Administration</b> <sup>[2]</sup>	Mice (n=9 per group; overnight fast) receive Asunaprevir (ASV) by oral gavage (5 mg/kg; vehicle of PEG-400-ethanol, 9:1). Blood samples (-0.2 mL) are obtained by retro-orbital bleeding at 0.25, 0.5, 1, 3, 6, 8, and 24 h after dosing. Within each group, three animals are bled at 0.25, 3, and 24 h, three at 0.5 and 6 h, and three at 1 and 8 h, resulting in a composite pharmacokinetic profile. Livers and brains are also removed from mice at the terminal sampling points. Rats (n=3 per group; overnight fast) receive ASV (amorphous free acid) by oral gavage (3, 5, 10, and 15 mg/kg) in PEG-400-ethanol (9:1). Serial blood samples (-0.3 mL) are obtained from the jugular vein predosing (0 h) and at 0.25, 0.5, 0.75, 1, 2, 4, 6, 8, 24, and 48 h postdosing. To assess tissue exposure, rats are orally administered ASV (5 or 15 mg/kg, same vehicle as above), and blood, liver, and heart samples from two rats/group are obtained at 0.17, 0.5, 1, 2, 4, 6, 8, 24, 48, and 72 h after dosing. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

## CUSTOMER VALIDATION

- Nature. 2020 Oct;586(7829):407-411.
- Cell. 2019 Aug 22;178(5):1145-1158.e20.
- Nat Methods. 2018 Jul;15(7):519-522.
- Signal Transduct Target Ther. 2021 May 29;6(1):212.
- Nat Neurosci. 2020 Feb;23(2):281-292.

See more customer validations on [www.MedChemExpress.com](http://www.MedChemExpress.com)

---

## REFERENCES

- [1]. Pelosi LA, et al. Effect on HCV Replication by Combinations of Direct Acting Antivirals Including NS5A Inhibitor BMS-790052. *Antimicrob Agents Chemother.* 2012 Jul 30.
- [2]. McPhee F, et al. Preclinical Profile and Characterization of the Hepatitis C Virus NS3 Protease Inhibitor Asunaprevir (BMS-650032). *Antimicrob Agents Chemother.* 2012 Aug 6.
- [3]. McPhee F, et al. Resistance analysis of the hepatitis C virus NS3 protease inhibitor asunaprevir. *Antimicrob Agents Chemother.* 2012 Jul;56(7):3670-81.
- [4]. Pasquinelli C, et al. Single- and multiple-ascending-dose studies of the NS3 protease inhibitor asunaprevir in subjects with or without chronic hepatitis C. *Antimicrob Agents Chemother.* 2012 Apr;56(4):1838-44.
- [5]. Qi Sun, et al. Bardoxolone and bardoxolone methyl, two Nrf2 activators in clinical trials, inhibit SARS-CoV-2 replication and its 3C-like protease. *Signal Transduct Target Ther.* 2021 May 29;6(1):212.
- 

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

Tel: 609-228-6898

Fax: 609-228-5909

E-mail: [tech@MedChemExpress.com](mailto:tech@MedChemExpress.com)

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA