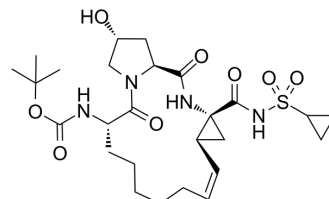


## ITMN 4077

<b>Cat. No.:</b>	HY-I0179		
<b>CAS No.:</b>	790305-05-4		
<b>Molecular Formula:</b>	C <sub>26</sub> H <sub>40</sub> N <sub>4</sub> O <sub>8</sub> S		
<b>Molecular Weight:</b>	568.68		
<b>Target:</b>	HCV Protease		
<b>Pathway:</b>	Anti-infection; Metabolic Enzyme/Protease		
<b>Storage:</b>	Powder	-20°C	3 years
	In solvent	-80°C	6 months
		-20°C	1 month



### SOLVENT & SOLUBILITY

#### In Vitro

DMSO : ≥ 100 mg/mL (175.85 mM)  
 \* "≥" means soluble, but saturation unknown.

Concentration	Solvent	Mass		
		1 mg	5 mg	10 mg
Preparing Stock Solutions	1 mM	1.7585 mL	8.7923 mL	17.5846 mL
	5 mM	0.3517 mL	1.7585 mL	3.5169 mL
	10 mM	0.1758 mL	0.8792 mL	1.7585 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 (4.40 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)  
 Solubility: ≥ 2.5 mg/mL (4.40 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% corn oil  
 Solubility: ≥ 2.5 mg/mL (4.40 mM); Clear solution

### BIOLOGICAL ACTIVITY

#### Description

ITMN 4077 is a macrocyclic inhibitor against Hepatitis C Virus (HCV) NS3 protease (EC<sub>50</sub>: 2131 nM)<sup>[1][2]</sup>.

#### IC<sub>50</sub> & Target

HCV NS3 protease<sup>[2]</sup>

### REFERENCES

---

[1]. Rajagopalan R, et al. Inhibition and binding kinetics of the hepatitis C virus NS3 protease inhibitor ITMN-191 reveals tight binding and slow dissociative behavior. *Biochemistry*. 2009 Mar 24;48(11):2559-68.

[2]. Jiang Y, et al. Discovery of danoprevir (ITMN-191/R7227), a highly selective and potent inhibitor of hepatitis C virus (HCV) NS3/4A protease. *J Med Chem*. 2014 Mar 13;57(5):1753-69.

---

**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