

**Catalog # 10-5087**

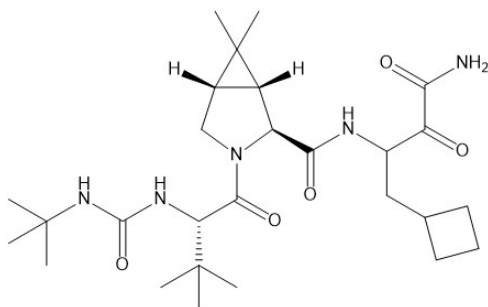
**Boceprevir**

CAS# 394730-60-0

(1R,2S,5S)-N-[3-amino-1-(cyclobutylmethyl)-2,3-dioxopropyl]-3-[(2S)-2-[[[(1,1-dimethyl-ethyl)amino]carbonyl]amino]-3,3-azabicyclo[3.1.0]hexane-2-carboxamide

SCH 503034

Lot # X109175



Boceprevir (394730-60-0) directly inhibits Hepatitis C virus (HCV) NS3 protease (overall binding constant for formation of covalent adduct,  $K_i^* = 14$  nM; initial inhibition constant  $K_i = 7.8$   $\mu$ M). This blocks NS3 autoactivation, and subsequent cleavage and maturation of other viral proteins necessary for replisome assembly. This reversible, slow-binding ketoamide also restores host interferon signaling obstructed by HCV, thus reactivating the immune response<sup>1</sup>. Recently, it was also found to inhibit the key SARS-CoV-2 protease, Mpro (3CLpro) *in vitro* ( $K_i = 1.18$   $\mu$ M) and in cells ( $EC_{50} = 1.9$   $\mu$ M, virus-induced cytopathic effects (CPE) assay).<sup>2</sup>

- 1) Malcom *et al.* (2006), SCH 503034, a Mechanism-Based Inhibitor of Hepatitis C Virus NS3 Protease, Suppresses Polyprotein Maturation and Enhances the Antiviral Activity of Alpha Interferon in Replicon Cells; *Antimicrob. Agents Chemother.*, **50** 1013
- 2) Ma *et al.* (2020), Boceprevir, GC-376, and Calpain Inhibitors II, XII Inhibit SARS-CoV-2 Viral Replication by Targeting the Viral Main Protease; *bioRxiv*, Preprint May 8, DOI 1101/2020.04.20.051581

**PHYSICAL DATA**

Molecular Weight: 519.68  
Molecular Formula: C<sub>27</sub>H<sub>45</sub>N<sub>5</sub>O<sub>5</sub>  
Purity: 98% by TLC  
NMR: (Conforms)  
Solubility: DMSO (up to 15 mg/ml with warming)  
Physical Description: White or off-white solid  
Storage and Stability: Store as supplied desiccated at -20°C for up to 2 years from the date of purchase. Solutions in DMSO may be stored at -20°C for up to 3 months.

**Materials provided by Focus Biomolecules are for laboratory research use only and are not intended for human or veterinary applications.**