MOLNOVA
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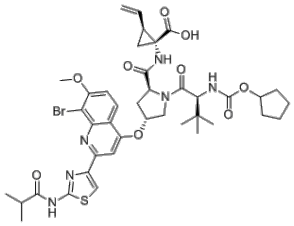
Datasheet (Version 1.0)

Product Name	:	Faldaprevir
Synonyms	:	BI 201335;BI201335;BI-201335
Cat No.	:	M15999
CAS Number	:	801283-95-4
Molecular Formula	:	C40H49BrN6O9S
Formula Weight	:	869.83



Chemical Name	:	(1R,2S)-1-[[(2S,4R)-4-[8-bromo-7-methoxy-2-[2-(2-methylpropanoylamino)-1,3-thiazol-4-yl]quinolin-4-yl]oxy-1-[(2S)-2-(cyclopentyloxycarbonylamino)-3,3-dimethylbutanoyl]pyrrolidine-2-carbonyl]amino]-2 ethenylcyclopropane-1-carboxylic acid
Description	:	A potent, selective noncovalent competitive inhibitor of HCV NS3/4A protease with Ki of 2.6 and 2.0 nM for GT1a and 1b NS3-NS4A protease, respectively; also shows Ki of 2 to 230 nM for HCV GT2 to 6, potently inhibits HCV RNA replication in vitro of 6.5 and 3.1 nM in genotype 1a and 1b replicon assays, respectively; possesses good ADME profile in vitro and pharmacokinetics in vivo.HCV Infection Phase 2 Clinical
Pathway	:	Microbiology/Virology
Target	:	HCV
Receptor	:	HCV
Solubility	:	——
SMILES	:	O=C([C@]1(NC([C@H]2N(C([C@@H](NC(OC3CCCC3)=O)C(C)(C)C)=O)C[C@H](OC4=CC(C5=CSC(NC(C(C)C)=O)=N5)=NC6=C(Br)C(OC)=CC=C46)C2)=O)[C@H](C=C)C1)O
Storage	:	(-20℃)
Stability	:	≥ 2 years
Reference	:	

1. Llinàs-Brunet M, et al. J Med Chem. 2010 Sep 9;53(17):6466-76.| 2. White PW, et al. Antimicrob Agents Chemother. 2010 Nov;54(11):4611-8.| 3. Manns MP, et al. J Hepatol. 2011 Jun;54(6):1114-22.| 4. Zeuzem S, et al. Gastroenterology. 2011 Dec;141(6):2047-55; quiz e14.