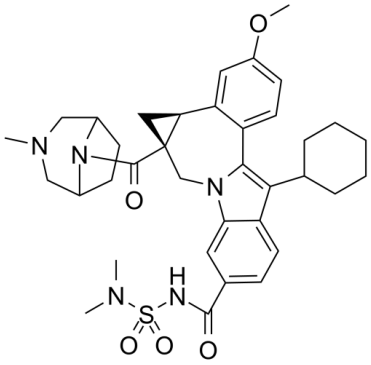
Data Sheet

Product Name:	Beclabuvir
Cat. No.:	CS-6041
CAS No.:	958002-33-0
Molecular Formula:	C36H45N5O5S
Molecular Weight:	659.84
Target:	HCV
Pathway:	Anti-infection
Solubility:	DMSO : ≥ 30 mg/mL (45.47 mM)



BIOLOGICAL ACTIVITY:

Beclabuvir is an allosteric inhibitor that binds to thumb site 1 of the hepatitis C virus (**HCV**) NS5B RNA-dependent RNA polymerase, and inhibits recombinant NS5B proteins from HCV genotypes 1, 3, 4, and 5 with **IC_{50}** of < 28 nM. IC50 & Target: IC50: < 28 nM (NS5B protein) **In Vitro:** Beclabuvir demonstrates additive or synergistic antiviral activity with pegIFN/RBV and in 2- or 3-drug combinations with a range of DAAs, such as HCV NS3 protease inhibitors, NS5A inhibitors' and/or nucleoside NS5B inhibitors[2]. **In Vivo:** The combination of beclabuvir with asunaprevir and daclatasvir achieves very high rates of viral eradication (about 90%) in patients infected with HCV genotype 1, which is the most common genotype worldwide[1].

References:

[1]. Gentile I, et al. Beclabuvir for the treatment of hepatitis C. Expert Opin Investig Drugs. 2015;24(8):1111-21

[2]. Tatum H, et al. A randomized, placebo-controlled study of the NS5B inhibitor beclabuvir with peginterferon/ribavirin for HCV genotype 1. J Viral Hepat. 2015 Aug;22(8):658-64.

CAIndexNames:

Cycloprop[d]indolo[2,1-a][2]benzazepine-9-carboxamide, 12-cyclohexyl-N-[(dimethylamino)sulfonyl]-4b,5,5a,6-tetrahydro-3-methoxy-5a-[(3-methyl-3,8-diazabicyclo[3.2.1]oct-8-yl)carbonyl]-, (4bS,5aR)-

SMILES:

O=C(N1C2CCC1CN(C)C2)[C@@]3(CN4C5=C(C6CCCCC6)C7=CC=C(C(NS(N(C)C)(=O)=O)=O)C=C47)[C@H](C8=CC(OC)=CC=C85)C3

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

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