Tegobuvir

Cat. No.: HY-10544

CAS No.: 1000787-75-6

Molecular Formula: $C_{25}H_{14}F_7N_5$

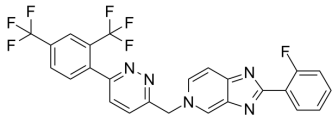
Molecular Weight: 517.4

Target: HCV

Pathway: Anti-infection

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 50 mg/mL (96.64 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	1.9327 mL	9.6637 mL	19.3274 mL
5 mM	0.3865 mL	1.9327 mL	3.8655 mL
10 mM	0.1933 mL	0.9664 mL	1.9327 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.75 mg/mL (5.32 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.75 mg/mL (5.32 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Tegobuvir is a specific, covalent inhibitor of the HCV NS5B polymerase.

In Vitro

Tegobuvir rapidly increases the proportion of replicons with the Y448H mutation in a dose-dependent manner. After 3 days of treatment, 1.2%, 6.8%, and > 50% of the replicon population expresses Y448H with the use of Tegobuvir at 1, 10, and 20 times its 50% effective concentration, respectively[1]. Tegobuvir exerts anti-HCV activity utilizing a unique chemical activation and subsequent direct interaction with the NS5B protein. Treatment of HCV subgenomic replicon cells with Tegobuvir results in a modified form of NS5B with a distinctly altered mobility on a SDS-PAGE gel[2]. Tegobuvir is potent in GT1a and 1b with mean EC_{50}s of 19.8 and 1.5 nM respectively. For genotype 3a, 4a, and 6a Con chimeras, tegobuvir EC_{50}s are all greater than 100 nM. The F445C NS5B mutations in GT3a, 4a, and 6a chimeric replicons restore tegobuvir potency to EC_{50}

levels comparable to GT1a[3].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Cell Assay [2]

Replicon-containing cells are trypsinized and seeded in cell culture media without G418 in white 96-well plates for EC_{50} analysis. Stable replicon carrying cell lines are seeded at a density of 5,000 cells per well. Serial threefold dilutions (10 concentrations) of compounds are performed in DMSO followed by further dilution in cell culture media and subsequent addition to cell plates. Compound-treated cells are incubated 72 hours at 37°C in a 5% CO_2 incubator.

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Proc Natl Acad Sci U S A. 2017 Feb 21;114(8):1922-1927.
- Antimicrob Agents Chemother. 2019 May 24;63(6). pii: e00003-19.
- Antiviral Res. 2019 Oct;170:104570.
- Biochem Biophys Res Commun. 2016 Jan 22;469(4):930-5.

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REFERENCES

[1]. Bae AS, et al. Allele-specific real-time PCR system for detection of subpopulations of genotype 1a and 1b hepatitis C NS5B Y448H mutant viruses in clinical samples. J Clin Microbiol. 2011 Sep;49(9):3168-74.

[2]. Hebner CM, et al. The HCV non-nucleoside inhibitor Tegobuvir utilizes a novel mechanism of action to inhibit NS5B polymerase function. PLoS One. 2012;7(6):e39163.

[3]. Wong KA, et al. Tegobuvir (GS-9190) potency against HCV chimeric replicons derived from consensus NS5B sequences from genotypes 2b, 3a, 4a, 5a, and 6a. Virology. 2012 Jul 20;429(1):57-62.

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

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