HCV-IN-38

Cat. No.: HY-115989

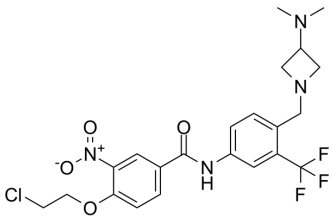
Molecular Formula: $C_{22}H_{24}ClF_3N_4O_4$

Molecular Weight: 500.9

Target: HCV

Pathway: Anti-infection

Storage: Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description

HCV-IN-38 is a potent, selective and orally active HCV inhibitor (EC_{50}=15 nM, SI=431). HCV-IN-38 has high anti-HCV activity and low cytotoxicity. HCV-IN-38 has a good safety and oral pharmacokinetic profile[1].

IC_{50} & Target

EC_{50}: 15 nM (HCV) in Huh7.5 cells[1]

In Vitro

HCV-IN-38 (compound 80) (0-20 μM; 72 hours) exhibits high anti-HCV activity with EC_{50}=15 nM and low cytotoxicity with CC_{50} =6.47 μM in Huh7.5 cells[1].

HCV-IN-38 (2 μM; 2 hours) has moderate permeability ($0.5 < P_{app} < 2.5$ ($\times 10^{-6}$ cm/s))[1].

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

Cell Cytotoxicity Assay

Cell Line:	Huh7.5 cells[1]
Concentration:	0-20 μM
Incubation Time:	72 hours
Result:	Exhibited low cytotoxicity with CC_{50}=6.47 μM.

In Vivo

HCV-IN-38 (2 μM; 4 hours) has decent plasma stability ($t_{1/2, rat}$=16.9 h and $t_{1/2, human}$=19.9 h)[1].

HCV-IN-38 (2 mg/kg for i.p., 10 mg/kg for p.o., single) exhibits satisfying PK properties with an oral total exposure (AUC) of 1502 ng h/mL, medium in vivo clearance (38.3 mL/min/kg), C_{max} of 452 ng/mL, and moderate bioavailability of 34%[1].

HCV-IN-38 (50-200 mg/kg; i.p., single) has modest safety profiles with LD_{50} values higher than 150 mg/kg[1].

Pharmacokinetic Parameters of HCV-IN-38 in Sprague-Dawley rats[1].

	IV (2 mg/kg)	PO (10 mg/kg)
$AUC_{0\text{-last}}$ (ng·h/mL)	889 ± 179	1502 ± 342
$AUC_{0\text{-inf}}$ (ng·h/mL)	898 ± 184	1525 ± 360

$MRT_{0\text{-last}}$ (h)	1.36 ± 0.182	2.95 ± 0.276
$MRT_{0\text{-inf}}$ (h)	1.45 ± 0.211	3.10 ± 0.290
C_{max} (ng/mL)		452 ± 149
$T_{1/2}$ (h)	1.24 ± 0.101	1.90 ± 0.492
T_{last} (h)	8.00	12.0
T_{max} (h)		1.00
Vd_{ss} (L/kg)	3.26 ± 0.426	
Cl (mL/min/kg)	38.3 ± 8.89	
F (%)	34	

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Animal Model:	SD rats (180-220 g, n=3)[1]
Dosage:	2 or 10 mg/kg
Administration:	i.v. and p.o., single (Pharmacokinetic Analysis)
Result:	Exhibited satisfying PK properties with an oral total exposure (AUC) of 1502 ng h/mL, medium in vivo clearance (38.3 mL/min/kg), C_{max} of 452 ng/mL, and moderate bioavailability of 34%.

Animal Model:	Kunming mice (n=6)[1]
Dosage:	50, 100, 150, and 200 mg/kg
Administration:	i.p., single
Result:	Demonstrated modest safety profiles with LD_{50} values higher than 150 mg/kg.

REFERENCES

[1]. Liu Y, et al. Synthesis and structure-activity relationship study of new biaryl amide derivatives and their inhibitory effects against hepatitis C virus. Eur J Med Chem. 2022;228:114033.

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

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