TMC647055 Choline salt

Cat. No.: HY-15591A

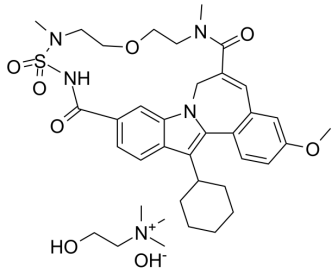
Molecular Formula: $C_{37}H_{53}N_5O_8S$

Molecular Weight: 727.91

Target: HCV

Pathway: Anti-infection

Storage: 4°C, sealed storage, away from moisture
* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 62.5 mg/mL (85.86 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.3738 mL	6.8690 mL	13.7380 mL
	5 mM	0.2748 mL	1.3738 mL	2.7476 mL
	10 mM	0.1374 mL	0.6869 mL	1.3738 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
Solubility: ≥ 2.08 mg/mL (2.86 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

TMC647055 (Choline salt) is a potent nonnucleoside NS5B polymerase inhibitor of HCV replication. TMC647055 Choline salt has potent HCV combine activity with an IC_{50} value of 82 nM. TMC647055 Choline salt can be used for the research of Hepatitis C virus (HCV)[1][2].

IC_{50} & Target

EC90: 0.3 μM (Huh7-Luc cell)[1].
EC50: 82 nM (HCV)[2]

In Vitro

TMC647055 (Choline salt) has antiviral activity with an EC_{90} value of 0.3 μM in Huh7-Luc cells[1].
TMC647055 Choline salt has potent combine activity with an EC_{50} value of 82 nM in cellular HCV assays[2].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

TMC647055 Choline salt (compound 18a) (2 mg/kg, iv.; 10mg/kg, po.) shows an acceptable PK profile, characterized by high oral bioavailability and high systemic exposure after single oral dosing of 10 mg/kg, combined with a moderate plasma clearanceand low volume of distribution[2].

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

Animal Model:	Rats[2]
Dosage:	2 mg/kg; 10mg/kg
Administration:	2 mg/kg, iv.; 10mg/kg, po.; singel
Result:	

No.	Cl (L/h/kg)	C_{max}(ng/mL)	[Liver] (ng/mL)	L/P	F (%)
TMC647055 (compound 18a)	3.2	440	7800	46	☒66

CUSTOMER VALIDATION

- Antiviral Res. 2019 Oct;170:104570.

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REFERENCES

[1]. Sandrine Vendeville, et al. Finger loop inhibitors of the HCV NS5b polymerase. Part II. Optimization of tetracyclic indole-based macrocycle leading to the discovery of TMC647055. Bioorg Med Chem Lett. 2012 Jul 1;22(13):4437-43.

[2]. Devogelaere B, et al. TMC647055, a potent nonnucleoside hepatitis C virus NS5B polymerase inhibitor with cross-genotypic coverage. Antimicrob Agents Chemother. 2012 Sep;56(9):4676-4684.

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