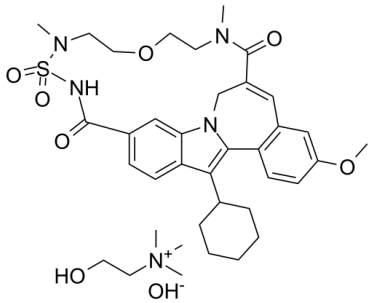
Data Sheet

Product Name:	TMC647055 (Choline salt)
Cat. No.:	CS-5338
Molecular Formula:	C37H53N5O8S
Molecular Weight:	727.91
Target:	HCV
Pathway:	Anti-infection
Solubility:	DMSO : ≥ 43 mg/mL (59.07 mM)



BIOLOGICAL ACTIVITY:

TMC647055 choline salt is a cell-permeating, selective HCV NS5B inhibitor, eliciting a mean IC50 of 34 nM, as assessed in the RdRp primer-dependent transcription assay. IC50 value: 34 nM [1] Target: HCV NS5B in vitro: TMC647055 is a novel and potent nonnucleoside inhibitor of the HCV NS5B RNA-dependent RNA polymerase. TMC647055 shows high selectivity for HCV when evaluated with a broad panel of human DNA and RNA viruses. TMC647055 shows median EC50 changes in the replicon assay of 9-, 3-, and 371-fold for L392I, V494A, and P495L, respectively, The median EC50 of TMC647055 on NS5B sequences derived from clinical isolates of genotypes 1a, 1b, 3a, 4a, and 6a ranged between 27 nM and 113 nM.[1]

PROTOCOL (Extracted from published papers and Only for reference)

Cell assay [1] Huh7-Luc replicon cells were seeded at a concentration of 3 × 105/10-cm dish and treated with different concentrations of compound in the presence of 250 μg/ml G418. TMC647055 concentrations of 375 nM, 750 nM, and 1.875 μM (approximately 5, 10, and 25 times the EC50, respectively) were used for genotype 1b resistance selection experiments. For the genotype 1a resistance selection experiments, 750 nM and 1,500 nM TMC647055 (approximately 5 and 10 times the EC50, respectively) were used. Medium was refreshed twice weekly, and fresh compound was added. Cells were subcultured when necessary, and significant cell death typically occurred after 2 to 3 weeks. Surviving cell colonies were individually picked or pooled and expanded. As soon as the quantity of cells obtained was sufficient, RNA was extracted and amplified and the NS5B region was sequenced by standard Sanger sequencing at a population level.

References:

[1]. 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.

CAIndexNames:

2,19-Methano-3,7:4,1-dimetheno-1H,11H-14,10,2,9,11,17-benzoxathiatetraazacyclodocosine-8,18(9H,15H)-dione, 27-cyclohexyl-12,13,16,17-tetrahydro-22-methoxy-11,17-dimethyl-, 10,10-dioxide, Choline salt

SMILES:

OCC[N+](C)(C)C.COC1=CC2=C(C=C1)C3=C(C4CCCCC4)C5=CC=C(C6=O)C=C5N3CC(C(N(C)CCOCCN(S(N6)(=O)=O)C)=O)=C2.[OH-]

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

Tel: 732-484-9848 Fax: 888-484-5008 E-mail: sales@ChemScene.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA