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## Product Data Sheet

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Product Name: TMC647055  
Cat. No.: GC13699

### Chemical Properties

Cas. No. 1204416-97-6

SMILES CN(C(C(CN1C2=C(C(C3CCCCC3)=C41)C=CC(/C(O)=N/S5(=O)=O)=C2)=CC6=C4C=CC(OC)=C6)=O)CCOCCN5C

Formula C<sub>32</sub>H<sub>38</sub>N<sub>4</sub>O<sub>6</sub>S

M.Wt 606.73

Solubility ≥ 72.8mg/mL in DMSO with gentle warming

Storage Store at -20°C

General For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution : ship with blue ice All other available size: ship with RT, or blue ice upon request.

Structure

### Background

TMC647055 is a potent and selective non-nucleoside inhibitor of the hepatitis C virus NS5B polymerase with EC<sub>50</sub> value of 82 nM [1].

Hepatitis C virus (HCV) NS5B polymerase is a RNA-dependant RNA-polymerase that is responsible for viral replication and plays an important role in HCV life cycle. HCV is a major cause of chronic liver disease and acute hepatitis, ultimately leading to liver failure, cirrhosis and hepatocellular carcinoma [1].

TMC647055 is a selective and cell-permeating HCV NS5B inhibitor. In RNA polymerase primer-dependent transcription assay, TMC647055 inhibited HCV NS5B polymerase with IC<sub>50</sub> value of 34 nM. In the Huh7-Luc cell line, TMC647055 inhibited the replication of genotype 1b replicon with EC<sub>50</sub> values of 77 and 139 nM measured with luciferase readout and qRT-PCR readout, respectively. TMC647055 exhibited high-affinity interaction with NS5B across all genotypes (except for genotype 2b) with median KD value < 35 nM. In Huh7-Luc replicon cells, TMC647055 (750 nM) reduced 30 cell colonies formation. Also, TMC647055 (1.5 μM and 3.75 μM) reduced HCV replicon RNA [2] [3].

### References:

- [1]. Vendeville S, Lin TI, Hu L, 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, 22(13): 4437-4443.
- [2]. Devogelaere B, Berke JM, Vijgen L, et al. TMC647055, a potent nonnucleoside hepatitis C virus NS5B polymerase inhibitor with cross-genotypic coverage. *Antimicrob Agents Chemother*, 2012, 56(9): 4676-4684.
- [3]. Cummings MD, Lin TI, Hu L, et al. Discovery and early development of TMC647055, a non-nucleoside inhibitor of the hepatitis C virus NS5B polymerase. *J Med Chem*, 2014, 57(5): 1880-1892.

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

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