

# **Product** Data Sheet

#### YM-53601

Cat. No.: HY-100313A CAS No.: 182959-33-7 Molecular Formula:  $C_{21}H_{22}CIFN_2O$ Molecular Weight: 372.86

Target: Farnesyl Transferase; HCV

Pathway: Metabolic Enzyme/Protease; Anti-infection

4°C, sealed storage, away from moisture Storage:

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

#### **SOLVENT & SOLUBILITY**

In Vitro

DMSO: 100 mg/mL (268.20 mM; ultrasonic and warming and heat to 60°C)

| Preparing<br>Stock Solutions | Solvent Mass<br>Concentration | 1 mg      | 5 mg       | 10 mg      |
|------------------------------|-------------------------------|-----------|------------|------------|
|                              | 1 mM                          | 2.6820 mL | 13.4099 mL | 26.8197 mL |
|                              | 5 mM                          | 0.5364 mL | 2.6820 mL  | 5.3639 mL  |
|                              | 10 mM                         | 0.2682 mL | 1.3410 mL  | 2.6820 mL  |

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

### **BIOLOGICAL ACTIVITY**

Description

 $YM-53601, a squalene \ synthase \ inhibitor, reduces \ plasma \ cholesterol \ and \ triglyceride \ levels \ in \ vivo \ ^{[1]}. \ YM-53601 \ inhibits$ squalene synthase derived from human hepatoma cells with an IC<sub>50</sub> of 79 nM. Lipid-lowering agent<sup>[2]</sup>. YM-53601 is also an inhibitor of farnesyl-diphosphate farnesyltransferase 1 (FDFT1) enzyme activity and abrogates HCV propagation<sup>[3]</sup>.

In Vitro

YM-53601 inhibits squalene synthase activities in hepatic microsomes from several species of rat, hamster, guinea-pig, rhesus monkey, and human-derived HepG2 cell with IC<sub>50</sub>s of 90, 170, 46, 45, and 79 nM, respectively<sup>[1]</sup>.

YM-53601 inhibits conversion of [3H] farnesyl diphosphate to  $[^3H]$  squalene by hamster liver squalene synthase with the IC $_{50}$ of 170 nM<sup>[2]</sup>.

YM-53601 (1 μM) potentiates the susceptibility of H35 cells to thapsigargin, lonidamine, and doxorubicin. YM-53601 (1 μM) reduces the mitochondrial cholesterol levels in both H35 and HepG2 cells<sup>[4]</sup>.

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

Cell Viability Assay<sup>[4]</sup>

| Cell Line:     | H35 and HepG2 cells |
|----------------|---------------------|
| Concentration: | 1 μΜ                |

| Incubation Time: | 24 hours  |  |
|------------------|---|--|
| Result:          | lt: Reduced the mitochondrial cholesterol levels in both H35 and HepG2 cells. |  |

#### In Vivo

YM-53601 suppresses cholesterol biosynthesis in rats  $(ED_{50}, 32 \text{ mg/kg})^{[1]}$ .

YM-53601 also reduces plasma non-HDL cholesterol levels in hamsters by approximately 70% at an oral dose of 50 mg/kg/day for 5 days<sup>[2]</sup>.

YM-53601 potentiates Doxorubicin-mediated hepatocellular carcinoma cells (HCC) growth arrest and cell death in vivo<sup>[4]</sup>. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

| Animal Model:   | Sprague-Dawley (SD) rats weighing 150-170 g <sup>[1]</sup>  |  |
|-----------------|---|--|
| Dosage:         | 6.25, 12.5, 25 or 50 mg/kg  |  |
| Administration: | Given a single p.o.   |  |
| Result:         | Inhibited cholesterol biosynthesis from acetate in a dose-dependent manner in rats. The ED $_{50}$ value for YM-53601 cholesterol biosynthesis inhibition is 32 $$ mg/kg. |  |
| Animal Model:   | Five- to six-week-old male BALB/c athymic (nu/nu) nude mice <sup>[4]</sup>  |  |
| Dosage:         | 15 mg/kg  |  |
| Administration: | 2 wk of daily treatment by p.o. gavage  |  |
| Result:         | Significantly decreased the intratumor cholesterol levels.  |  |

#### **CUSTOMER VALIDATION**

• Research Square Preprint. 2023 Jun 22.

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## **REFERENCES**

- [1]. T Ugawa, et al. YM-53601, a novel squalene synthase inhibitor, reduces plasma cholesterol and triglyceride levels in several animal species. Br J Pharmacol. 2000 Sep;131(1):63-70.
- [2]. Tsukasa Ishihara, et al. Syntheses of 3-ethylidenequinuclidine derivatives as squalene synthase inhibitors. Part 2: enzyme inhibition and effects on plasma lipid levels. Bioorg Med Chem. 2003 Aug 15;11(17):3735-45.
- $[3]. \ Eun-Mee\ Park,\ et\ al.\ Farnesyl-diphosphate\ farnesyltransferase\ 1\ regulates\ hepatitis\ C\ virus\ propagation.\ FEBS\ Lett.\ 2014\ May\ 2;588(9):1813-20.$
- [4]. Joan Montero, et al. Mitochondrial cholesterol contributes to chemotherapy resistance in hepatocellular carcinoma. Cancer Res. 2008 Jul 1;68(13):5246-56.

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

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA

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