Theaflavin 3,3'-digallate

Cat. No.: HY-N1992

CAS No.: 30462-35-2

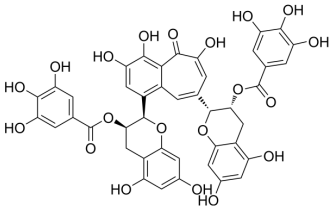
Molecular Formula: $C_{43}H_{32}O_{20}$

Molecular Weight: 868.7

Target: Virus Protease; HSV; HIV; Flavivirus

Pathway: Anti-infection

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



SOLVENT & SOLUBILITY

In Vitro

H_2O : ≥ 100 mg/mL (115.11 mM)
DMSO : 100 mg/mL (115.11 mM; Need ultrasonic)
* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	1.1511 mL	5.7557 mL	11.5115 mL
5 mM	0.2302 mL	1.1511 mL	2.3023 mL
10 mM	0.1151 mL	0.5756 mL	1.1511 mL

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

In Vivo

1. Add each solvent one by one: PBS
   Solubility: 50 mg/mL (57.56 mM); Clear solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (2.88 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (2.88 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Theaflavin 3,3'-digallate (TF-3) is a potent Zika virus (ZIKV) protease inhibitor with an IC_{50} of 2.3 μM. Theaflavin 3,3'-digallat directly binds to ZIKVpro (K_d=8.86 μM) and inhibits ZIKV replication. Theaflavin 3,3'-digallat inhibits the activity of gp41 and NS2B-3 protease and has antiviral activity against HSV and HIV-1[1]. Theaflavin 3,3'-digallate, the typical pigment in black tea, is a potent antitumor agent[2].

IC_{50} & Target	HSV	HIV-1

In Vitro

Theaflavin 3,3'-digallate (TF-3; 6.25, 12.5, 25 μM; 24 hours) markedly reduces viral RNA copy numbers and NS3, U87 MG protein expression in a dose-dependent manner[1].

Theaflavin 3,3'-digallate inhibits dose-dependently ZIKV replication in Vero E6 cells (EC_{50}=7.65 μM). Theaflavin 3,3'-digallate has minor cytotoxicity up to 40 μM in Vero E6 cells. Theaflavin 3,3'-digallate can inhibit the post-entry events of the ZIKV replication cycle from gene transcription and translation levels[1].

Theaflavin 3,3'-digallate is generally regarded as the effective component for the inhibitory effects against carcinogenesis without adverse side effects by affecting multiple signal transduction pathways, such as upregulating p53 and p21, inhibiting phosphorylation of the cell survival protein Akt and MAPK pathway, downregulation of NF-κB, shifting the ratio between pro-/antiapoptotic proteins. Theaflavin 3,3'-digallate causes a rapid and sustained decrease in phospho-ERK1/2 and -MEK1/2 protein expression. Theaflavin 3,3'-digallate inhibits HCT116 cell growth with an IC_{50} of 17.26 μM[2].

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

Western Blot Analysis[1]

Cell Line:	Vero E6 cells
Concentration:	6.25, 12.5, 25 μM
Incubation Time:	24 hours
Result:	Markedly reduced NS3, U87 MG protein expression in a dose-dependent manner.

CUSTOMER VALIDATION

- Front Pharmacol. 2021 Mar 23;12:648969.
- Microbiol Spectr. 2023 Sep 21;e0267123.
- Exp Ther Med. October 28, 2021.

See more customer validations on www.MedChemExpress.com

REFERENCES

[1]. Ding Y, et al. Pre-treated theaflavin-3,3'-digallate has a higher inhibitory effect on the HCT116 cell line. Food Nutr Res. 2017 Nov 15;61(1):1400340.

[2]. Xiangling Cui, et al. Identification of Theaflavin-3,3'-Digallate as a Novel Zika Virus Protease Inhibitor. Front Pharmacol. 2020 Oct 21;11:514313.

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