Theaflavin

Cat. No.: HY-N0243

CAS No.: 4670-05-7

Molecular Formula: $C_{29}H_{24}O_{12}$

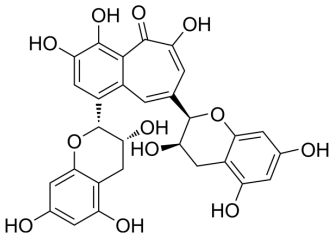
Molecular Weight: 564.49

Target: Influenza Virus; Endogenous Metabolite

Pathway: Anti-infection; Metabolic Enzyme/Protease

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 50 mg/mL (88.58 mM; Need ultrasonic)

H_2O : 2 mg/mL (3.54 mM; Need ultrasonic and warming)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	1.7715 mL	8.8576 mL	17.7151 mL
5 mM	0.3543 mL	1.7715 mL	3.5430 mL
10 mM	0.1772 mL	0.8858 mL	1.7715 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: 3 mg/mL (5.31 mM); Clear solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 3 mg/mL (5.31 mM); Clear solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: 3 mg/mL (5.31 mM); Suspended solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

Theaflavin is a suitable natural inhibitor against influenza A (H1N1) neuraminidase.

IC_{50} & Target

Influenza A (H1N1) virus[1]

In Vitro

Theaflavin, found in green tea, is observed to inhibit H1N1 NA proteins strongly supported by lowest docking energy. Theaflavin is a plant product traditionally used for treatment of influenza infection. Green tea is particularly rich in

polyphenolic compounds like Theaflavin. Theaflavin derivatives have shown pronounced antiviral activity. Theaflavin is found to interact with the amino acid residues like Arg118, Asp151, Asp 152, Arg193, Asp199, Asn344, and Arg430 of NA by forming hydrogen bonds[1].

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

CUSTOMER VALIDATION

- Acta Pharm Sin B. 2021 Jan;11(1):143-155.
- Int J Biol Sci. 2021 Mar 2;17(4):1050-1060.
- ACS Omega. 2024 May 17.

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REFERENCES

[1]. Sahoo M, et al. Identification of Suitable Natural Inhibitor against Influenza A (H1N1) Neuraminidase Protein by Molecular Docking. Genomics Inform. 2016 Sep;14(3):96-103.

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