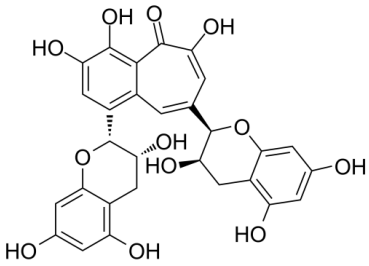
Data Sheet

Product Name:	Theaflavin
Cat. No.:	CS-5885
CAS No.:	4670-05-7
Molecular Formula:	C29H24O12
Molecular Weight:	564.49
Target:	Influenza Virus
Pathway:	Anti-infection
Solubility:	DMSO : 1.42 mg/mL (2.52 mM; Need ultrasonic and warming); H2O : 2 mg/mL (3.54 mM; Need ultrasonic and warming)



BIOLOGICAL ACTIVITY:

Theaflavin is a suitable natural inhibitor against influenza A (**H1N1**) neuraminidase. IC50 & 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].

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.

CAIndexNames:

5H-Benzocyclohepten-5-one, 1,8-bis[(2R,3R)-3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-2-yl]-3,4,6-trihydroxy-

SMILES:

O=C1C(O)=CC([C@@H]2[C@H](O)CC3=C(O)C=C(O)C=C3O2)=CC4=C([C@@H]5[C@H](O)CC6=C(O)C=C(O)C=C6O5)C=C(O)C(O)=C41

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

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