(±)-Alliin

Cat. No.: HY-126085

CAS No.: 17795-26-5

Molecular Formula: $C_6H_{11}NO_3S$

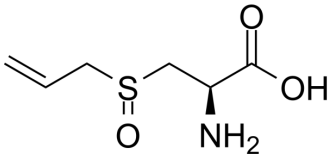
Molecular Weight: 177.22

Target: SARS-CoV

Pathway: Anti-infection

Storage:

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



SOLVENT & SOLUBILITY

In Vitro

H_2O : 125 mg/mL (705.34 mM; Need ultrasonic)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	5.6427 mL	28.2135 mL	56.4270 mL
	5 mM	1.1285 mL	5.6427 mL	11.2854 mL
	10 mM	0.5643 mL	2.8214 mL	5.6427 mL

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

BIOLOGICAL ACTIVITY

Description

(±)-Alliin is the main active component of garlic. (±)-Alliin is a putative inhibitor of the main protease of SARS-CoV-2 (M_{pro})[1].

In Vitro

Molecular docking is used to assess the binding stability of various drugs with SARS-CoV-2 main protease (Mpro).
(±)-Alliin is found to interact with SARS-CoV Mpro at Leu-167, Met-49 and Glu-166 with three H-bonds; for SARS-CoV-2 Mpro, the observed docking sites of (±)-Alliin are Cys-145, Met-49 and Glu-166 with three H-bonds[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Nucleic Acids Res. 2021 Jan 8;49(D1):D1113-D1121.
- Sci Rep. 2022 Jul 16;12(1):12197.

See more customer validations on www.MedChemExpress.com

REFERENCES

[1]. Bijun Cheng, et al. Discovery of Alliin as a Putative Inhibitor of the Main Protease of SARS-CoV-2 by Molecular Docking. Biotechniques

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