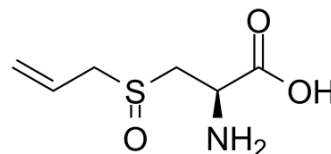


## (±)-Alliin

Cat. No.:	HY-126085
CAS No.:	17795-26-5
Molecular Formula:	C <sub>6</sub> H <sub>11</sub> NO <sub>3</sub> S
Molecular Weight:	177.22
Target:	SARS-CoV
Pathway:	Anti-infection
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



### BIOLOGICAL ACTIVITY

<b>Description</b>	(±)-Alliin is the main active component of garlic. (±)-Alliin is a putative inhibitor of the main protease of SARS-CoV-2 (M <sub>pro</sub> ) <sup>[1]</sup> .
<b>In Vitro</b>	Molecular docking is used to assess the binding stability of various drugs with SARS-CoV-2 main protease (M <sub>pro</sub> ). (±)-Alliin is found to interact with SARS-CoV M <sub>pro</sub> at Leu-167, Met-49 and Glu-166 with three H-bonds; for SARS-CoV-2 M <sub>pro</sub> , the observed docking sites of (±)-Alliin are Cys-145, Met-49 and Glu-166 with three H-bonds <sup>[1]</sup> . MCE has not independently confirmed the accuracy of these methods. They are for reference only.

### CUSTOMER VALIDATION

- Nucleic Acids Res. 2020 Nov 9;gkaa969.

See more customer validations on [www.MedChemExpress.com](http://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

**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](mailto:tech@MedChemExpress.com)

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA