

Investigation into SARS-CoV-2 Resistance of Compounds in Garlic Essential Oil

Bui Thi Phuong Thuy, Tran Thi Ai My, Nguyen Thi Thanh Hai, Le Trung Hieu, Tran Thai Hoa, Huynh Thi Phuong Loan, Nguyen Thanh Triet, Tran Thi Van Anh, Phan Tu Quy, Pham Van Tat, Nguyen Van Hue, Duong Tuan Quang,* Nguyen Tien Trung, Vo Thanh Tung, Lam K. Huynh, and Nguyen Thi Ai Nhung*



Cite This: *ACS Omega* 2020, 5, 8312–8320



Read Online

ACCESS |



Metrics & More



Article Recommendations



Supporting Information

ABSTRACT: Eighteen active substances, including 17 organosulfur compounds found in garlic essential oil (T), were identified by GC–MS analysis. For the first time, using the molecular docking technique, we report the inhibitory effect of the considered compounds on the host receptor angiotensin-converting enzyme 2 (ACE2) protein in the human body that leads to a crucial foundation about coronavirus resistance of individual compounds on the main protease (PDB6LU7) protein of SARS-CoV-2. The results show that the 17 organosulfur compounds, accounting for 99.4% contents of the garlic essential oil, have strong interactions with the amino acids of the ACE2 protein and the main protease PDB6LU7 of SARS-CoV-2. The strongest anticoronavirus activity is expressed in allyl disulfide and allyl trisulfide, which account for the highest content in the garlic essential oil (51.3%). Interestingly, docking results indicate the synergistic interactions of the 17 substances, which exhibit good inhibition of the ACE2 and PDB6LU7 proteins. The results suggest that the garlic essential oil is a valuable natural antivirus source, which contributes to preventing the invasion of coronavirus into the human body.



1. INTRODUCTION

Garlic (*Allium sativum* L.) (cf. Figure 1) is considered as an important herb thanks to its variety of uses, including either a common spice for family meals or a popular component in folk-medicine prescriptions.^{1,2} For thousands of years, garlic



Figure 1. Picture of garlic (*A. sativum* L.).

has been used as a medication for common colds, influenza, and other kinds of infections.^{3,4} Recent pharmacological studies indicate that essential oil of garlic is an exceptional source of organosulfur compounds, possessing strong antioxidant, antibacterial, antifungal, anticancer, and antimicrobial properties. The oil is also proven to be conducive to hypoglycemia, hypotension, antithrombotic, immunomodulatory, and prebiotic therapy. Besides, allicin is a typical reactive sulfur species found in the essential oil.⁵

Recently, many people have been infected with a novel coronavirus (SARS-CoV-2), and the death toll has reached thousands and been increasing day by day, which is a major problem in the world.⁶ Therefore, the demand to seek for natural and safe medicines to prevent coronavirus is of great concern for all scientists around the world. With abundant medicinal resources in Vietnam and the specific healing properties of garlic,⁷ we herein recommend a solution for the

Received: February 21, 2020

Accepted: March 20, 2020

Published: March 31, 2020

